TRIUMF McGill UNIVERSITY nEXO

Global ab initio calculations for exotic and heavy nuclei

Jason D. Holt
TRIUMF, Theory Department
ARIS 2023
June 7, 2023

Discovery, accelerated

NSERC CRSNG Arthur B. McDonald Canadian Astroparticle Physics Research Institute NRC·CNRC

Major RIB Facilities Worldwide

Next-generation RIB facilities: unprecedented era of nuclear science

Thousands of new isotopes to be produced: **How does our field maximize this opportunity?**

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Thousands of new isotopes to be produced: **Meaningful interaction with theory!**

$4-5B worldwide investment

What is the fundamental, exciting physics?

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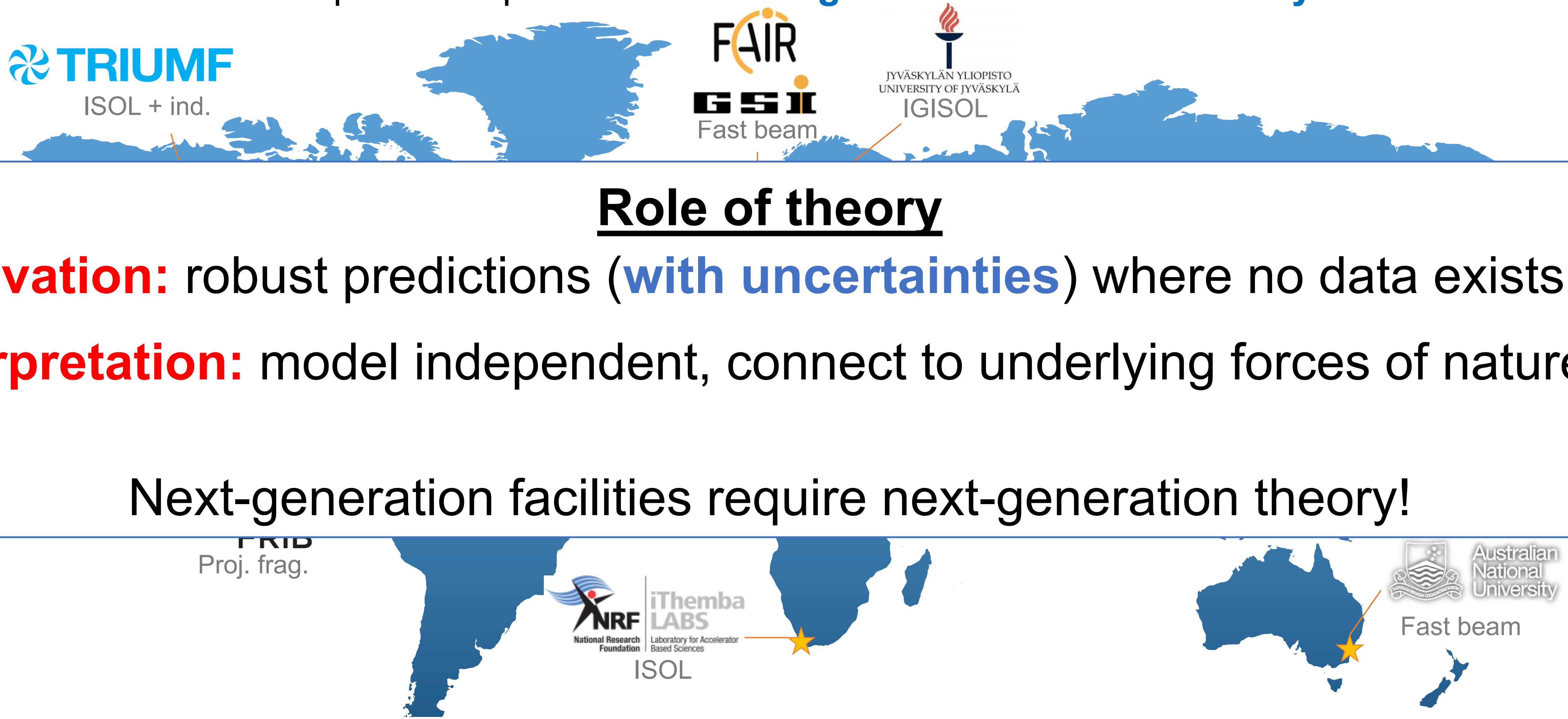


Role of theory

Motivation: robust predictions (**with uncertainties**) where no data exists

Interpretation: model independent, connect to underlying forces of nature

Next-generation facilities require next-generation theory!

$4-5B worldwide investment

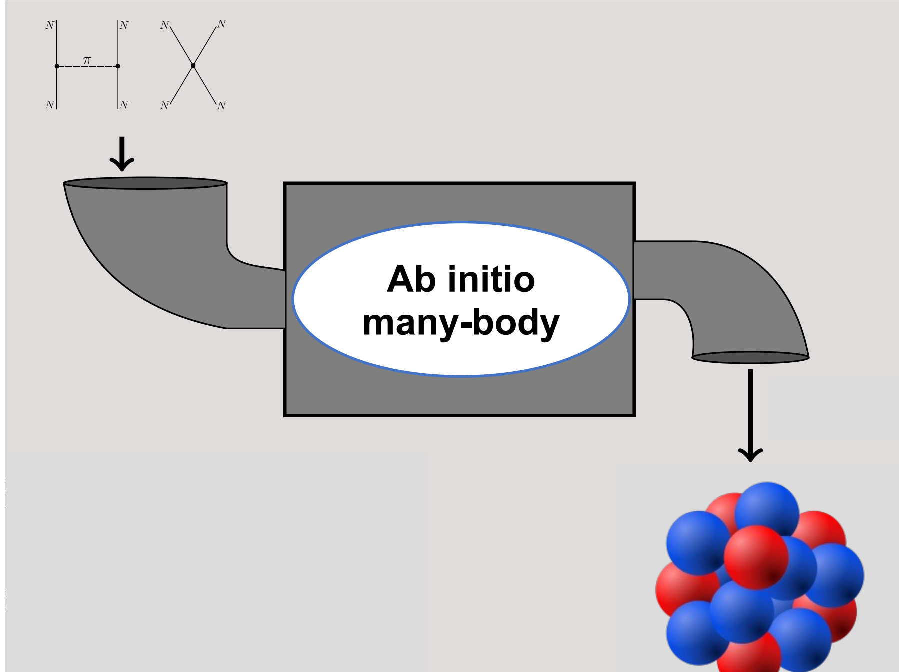
What is the fundamental, exciting physics?

Ab Initio Approach to Nuclear Structure

Aim of modern nuclear theory: develop unified *first-principles* picture of structure and reactions

(Approximately) solve nonrelativistic Schrödinger equation

$$H\psi_n = E_n\psi_n$$



Courtesy, S. R. Stroberg

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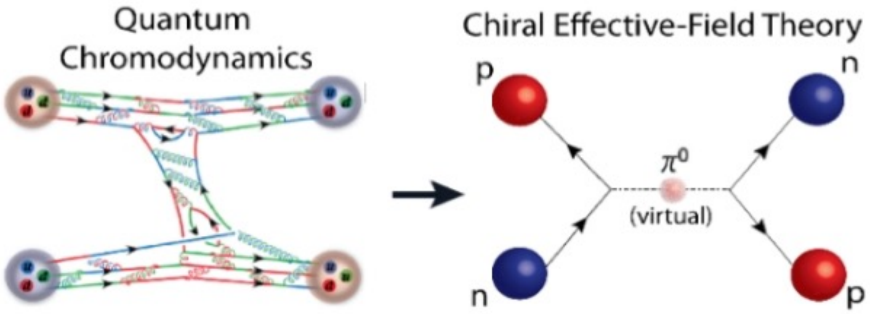
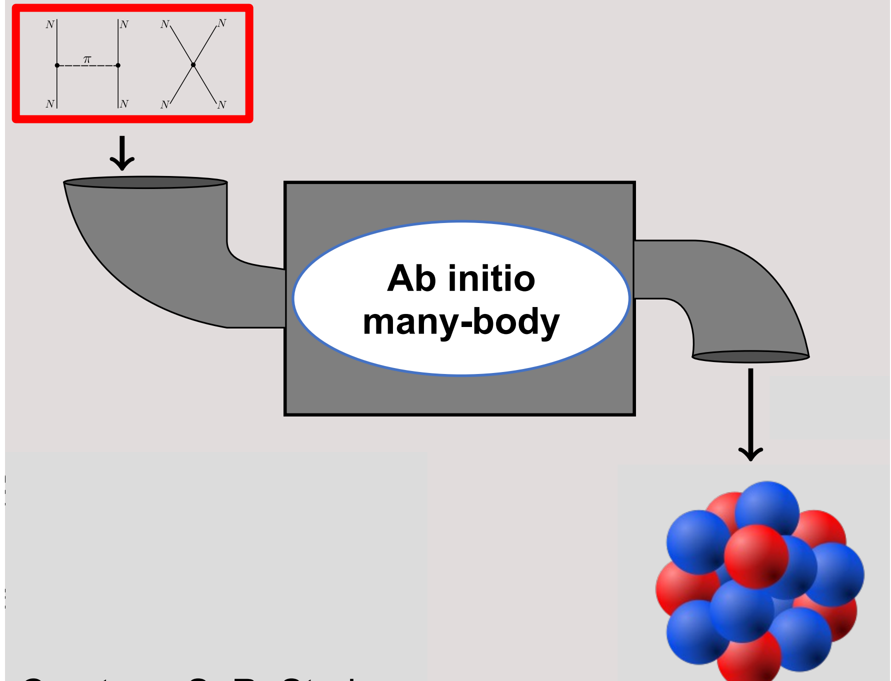




Courtesy, S. R. Stroberg

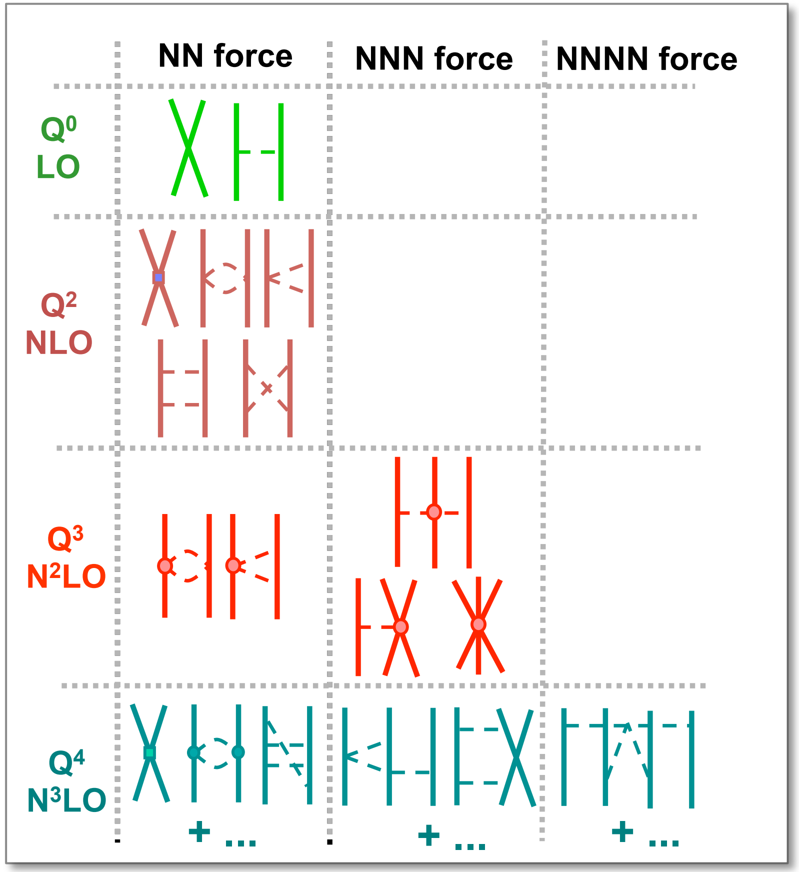
Chiral Effective Field Theory

Consistent treatment of
- 2N, 3N, 4N, … forces
- Electroweak physics

Quantifiable uncertainties

Interactions

1.8/2.0, N2LO$_{GO}$, N3LO$_{LNL}$
(2.0/2.0, N4LO$_{LNL}$)
34 non-implausible



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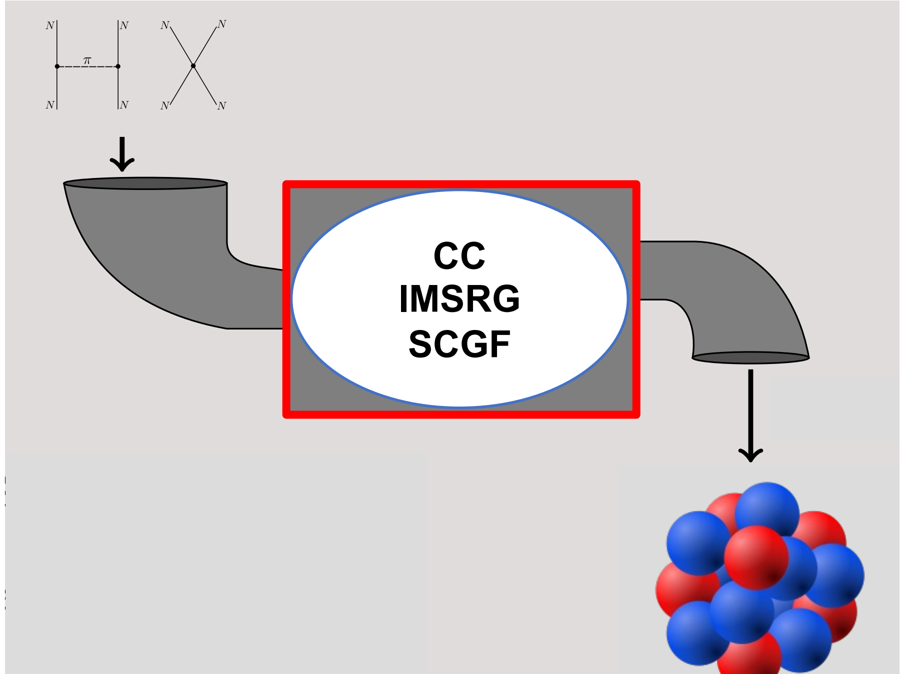
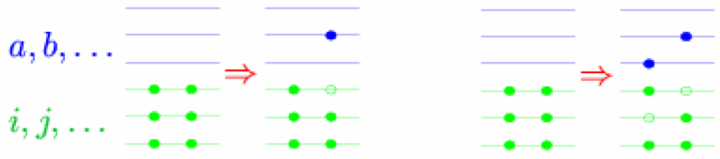


Courtesy, S. R. Stroberg

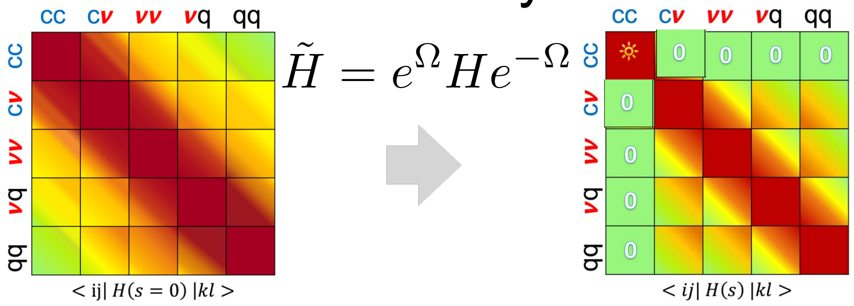
Ab Initio Cheat Sheet (polynomial scaling methods)

CC: Coupled cluster theory

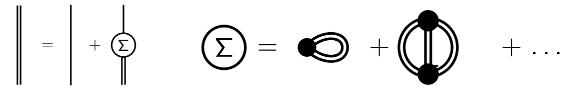


$$\begin{aligned} E &= \langle\Phi|\overline{H}|\Phi\rangle \\ 0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\ 0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle \\ \overline{H} &\equiv e^{-T}He^{T} = \left(He^{T}\right)_c \end{aligned}$$

IMSRG: In-medium similarity renormalization group



SCGF: Self-consistent Green's function



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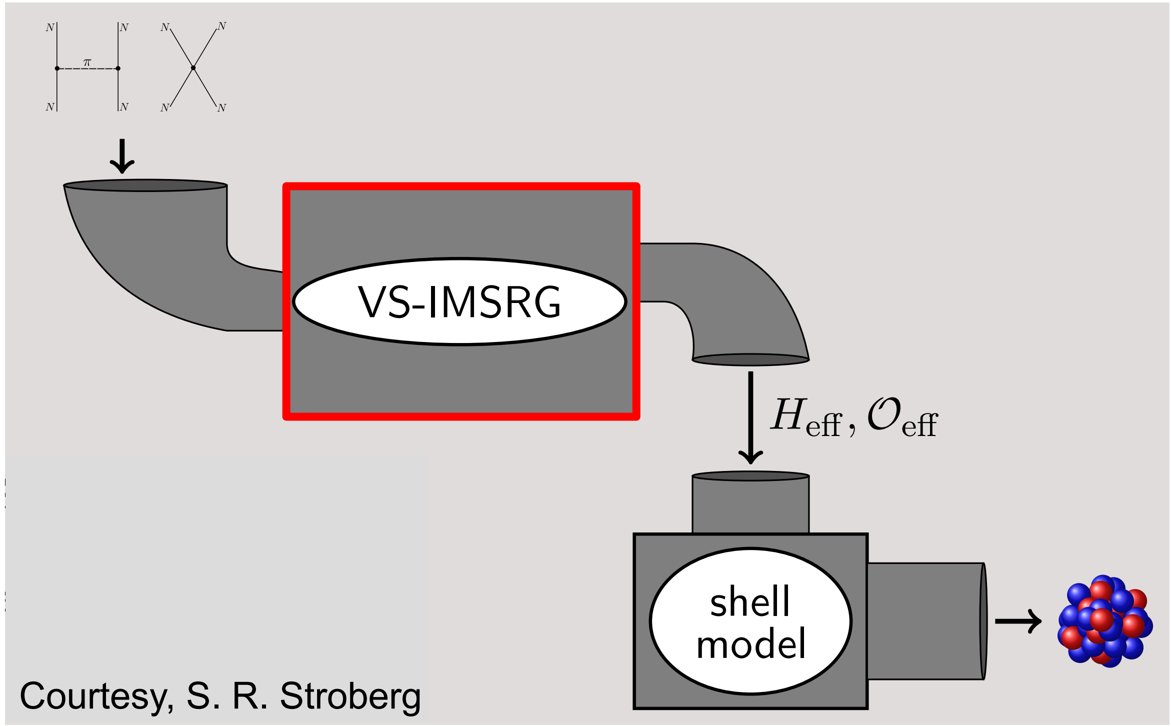

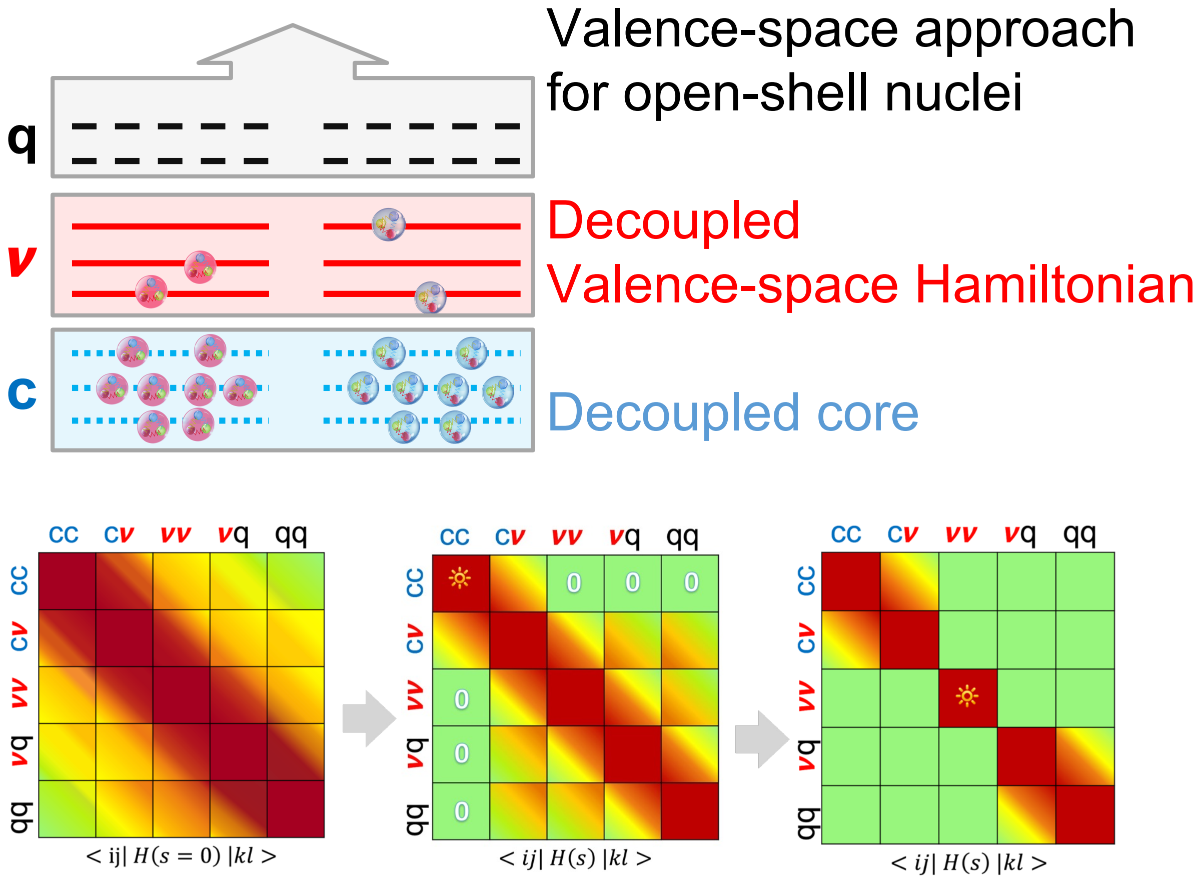

Extends ab initio to scope of traditional nuclear shell model

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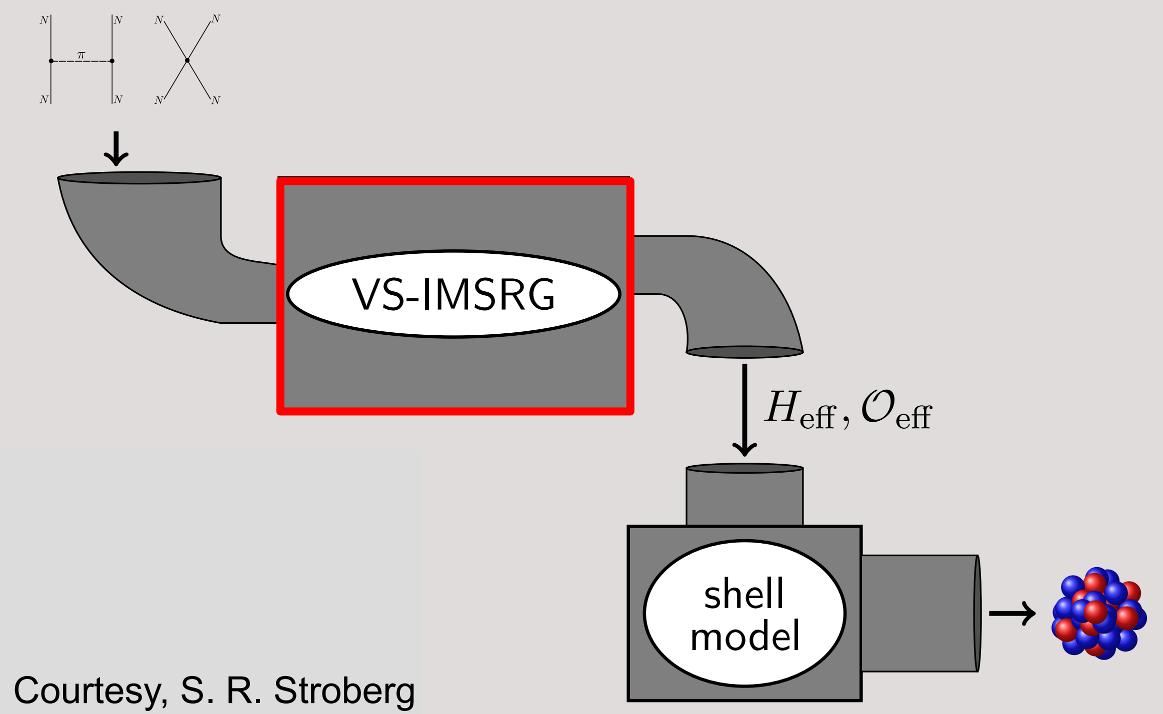


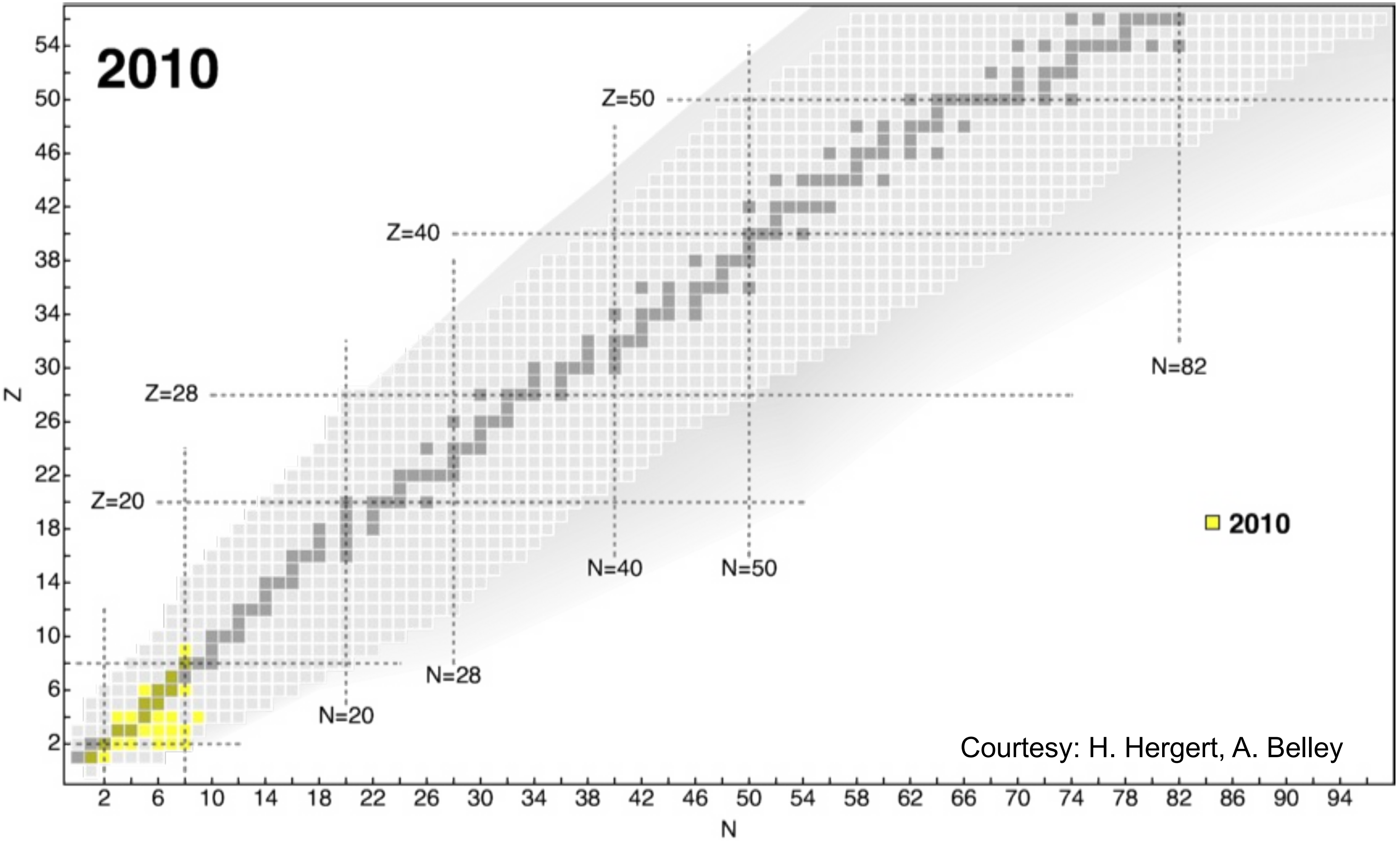
Courtesy, S. R. Stroberg

Methods Exact up to Truncations

- ✅ **Single-particle basis** $e_{\max} = 2n + l$
- ✅ **Storage limits of 3N forces** $e_1 + e_2 + e_3 \leq E_{3\max}$
- 🤷 **Many-body operators: e.g., CCSD(T), IMSRG(2)**

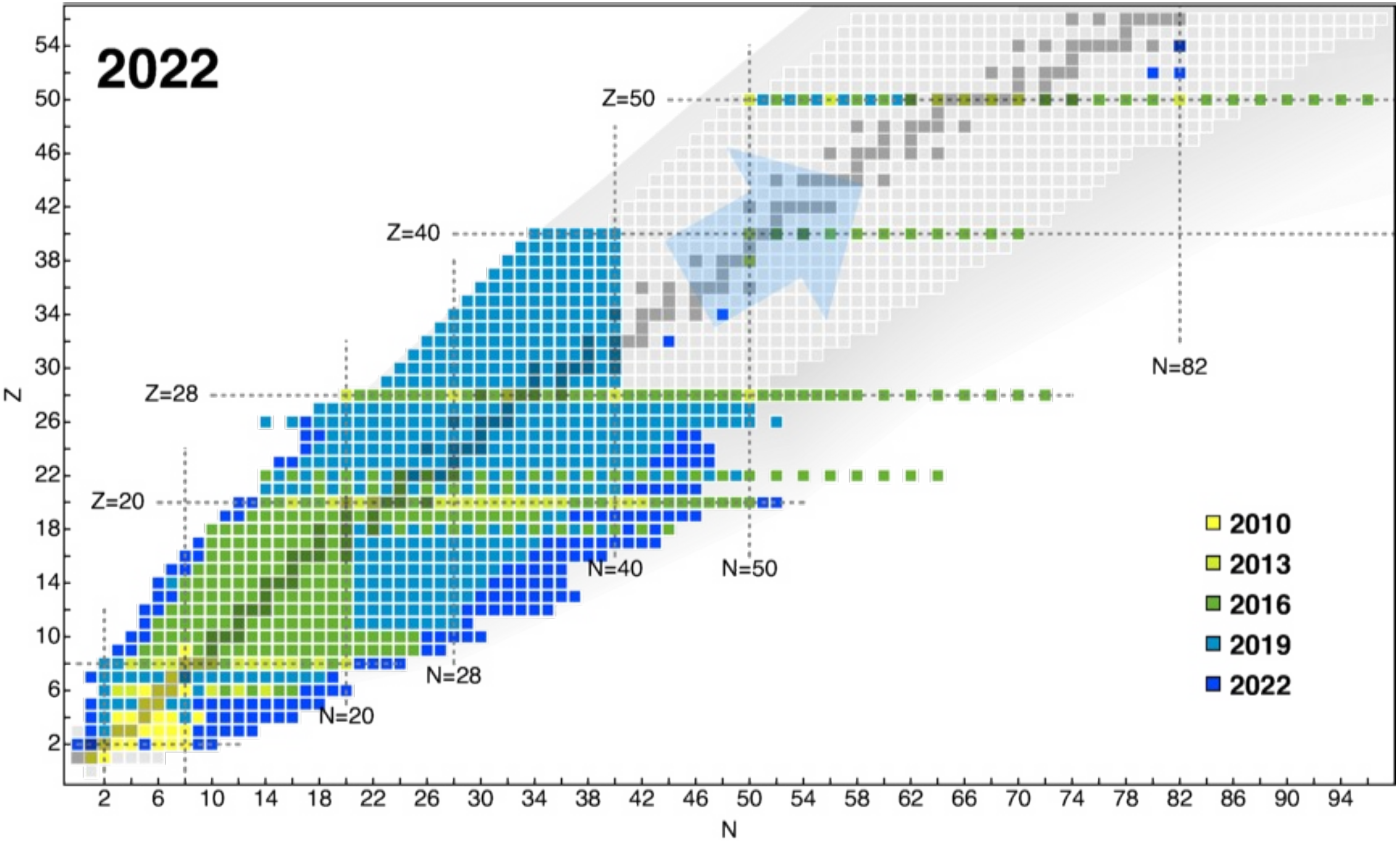
Progress of Ab Initio Theory Since 2010

2010: Limited capabilities for 3N forces; ^{16}O heaviest



Ab Initio Progress: How Heavy Can We Go?

Tremendous progress in ab initio reach, largely due to polynomially scaling methods!



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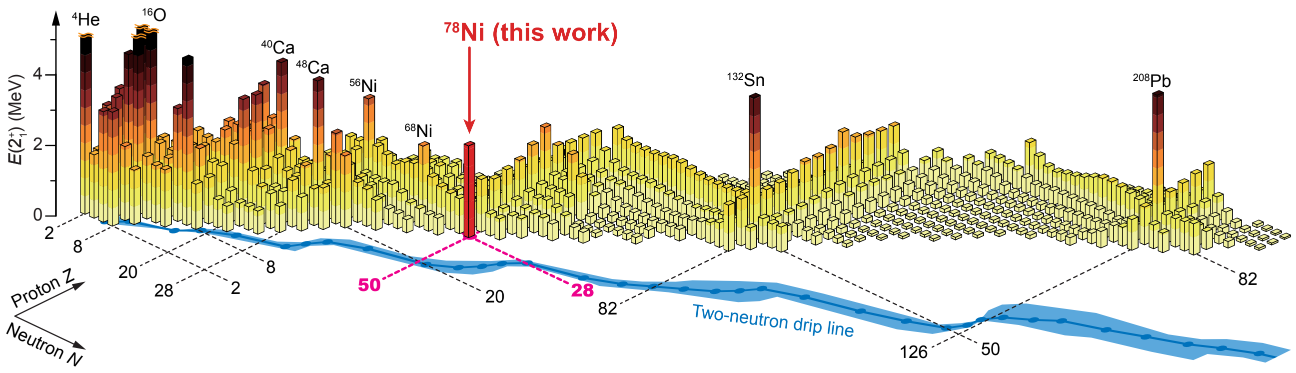
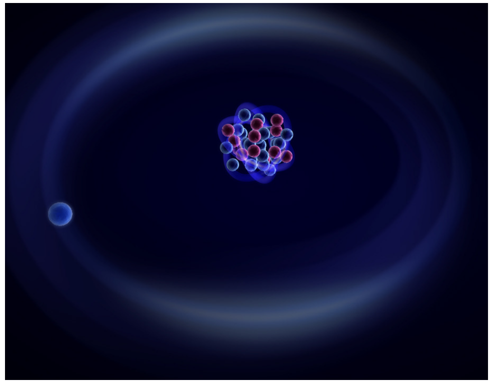
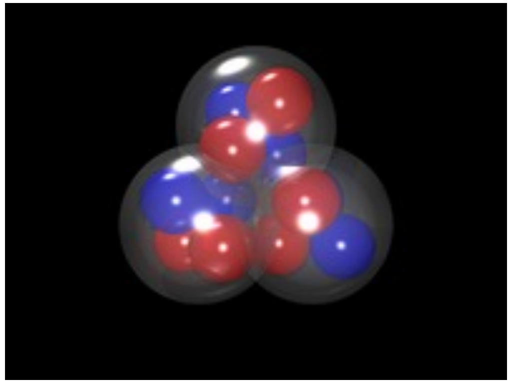
Major Questions in Nuclear Structure

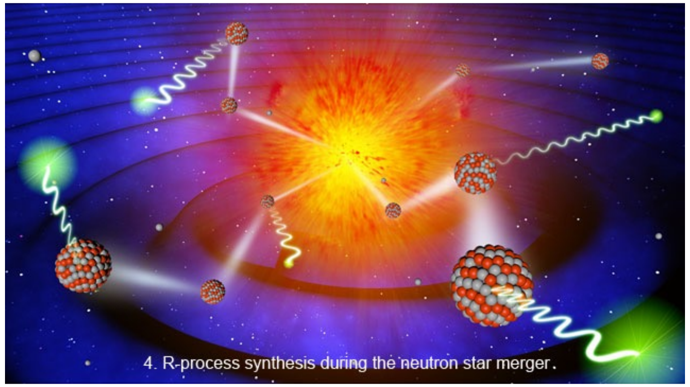


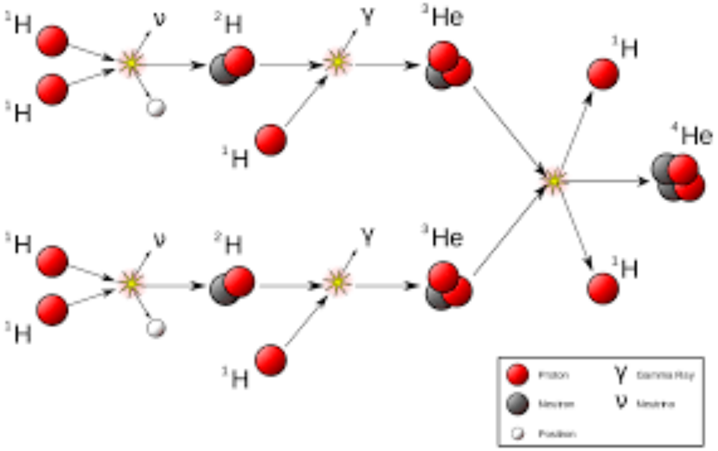


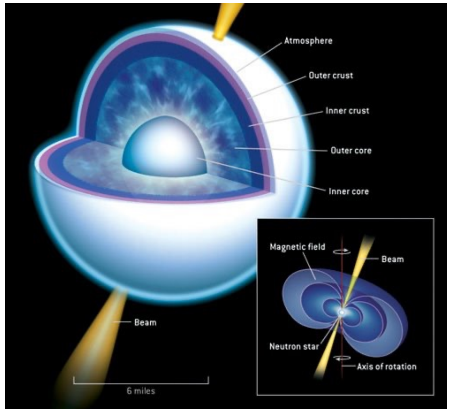


Limits of existence + formation/evolution of magic numbers

Nuclear skins/halos/clusters





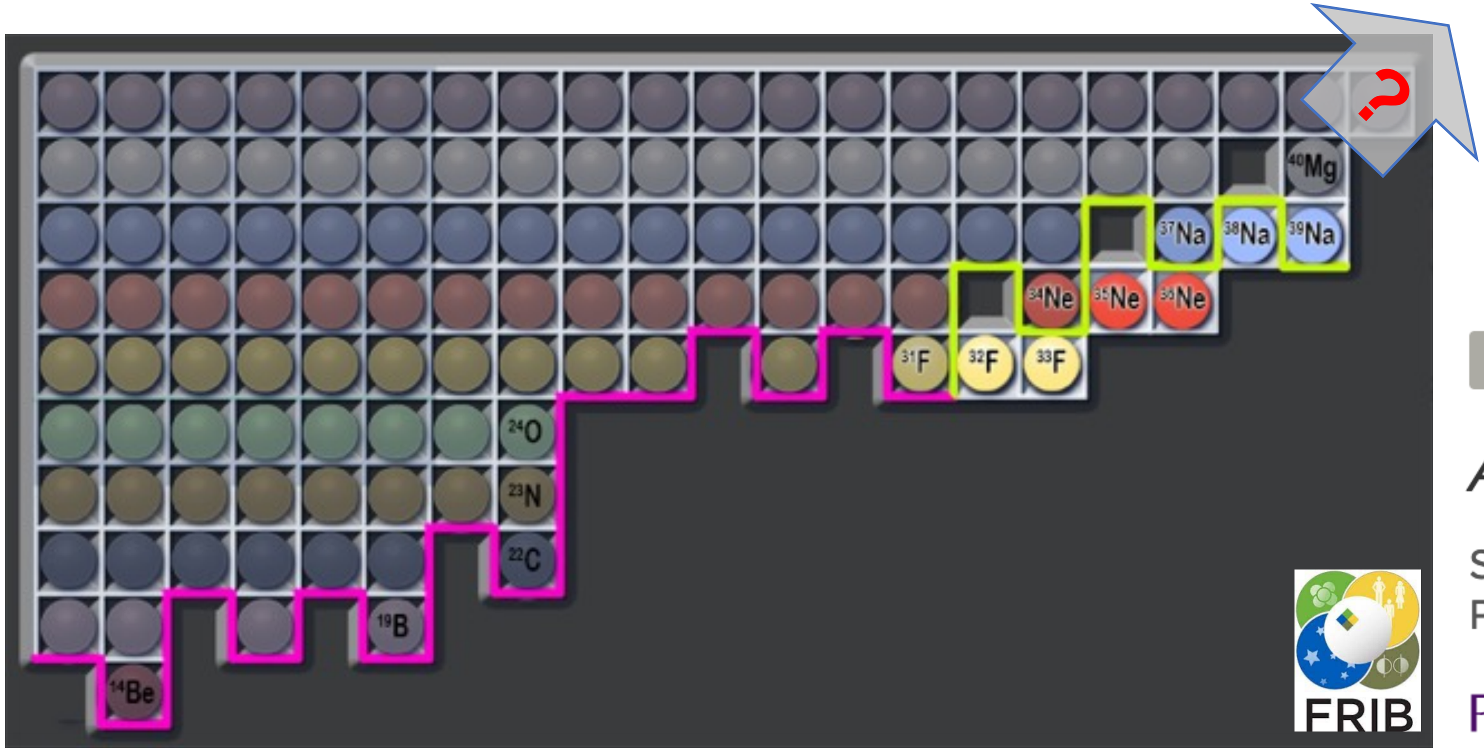


Heavy Nuclei + r-process

Continuum and nuclear reactions

Infinite matter/Neutron stars

Global Ab Initio Calculations: Proton/Neutron Driplines



Featured in Physics | Editors' Suggestion

Ab Initio Limits of Atomic Nuclei

S. R. Stroberg, J. D. Holt, A. Schwenk, and J. Simonis

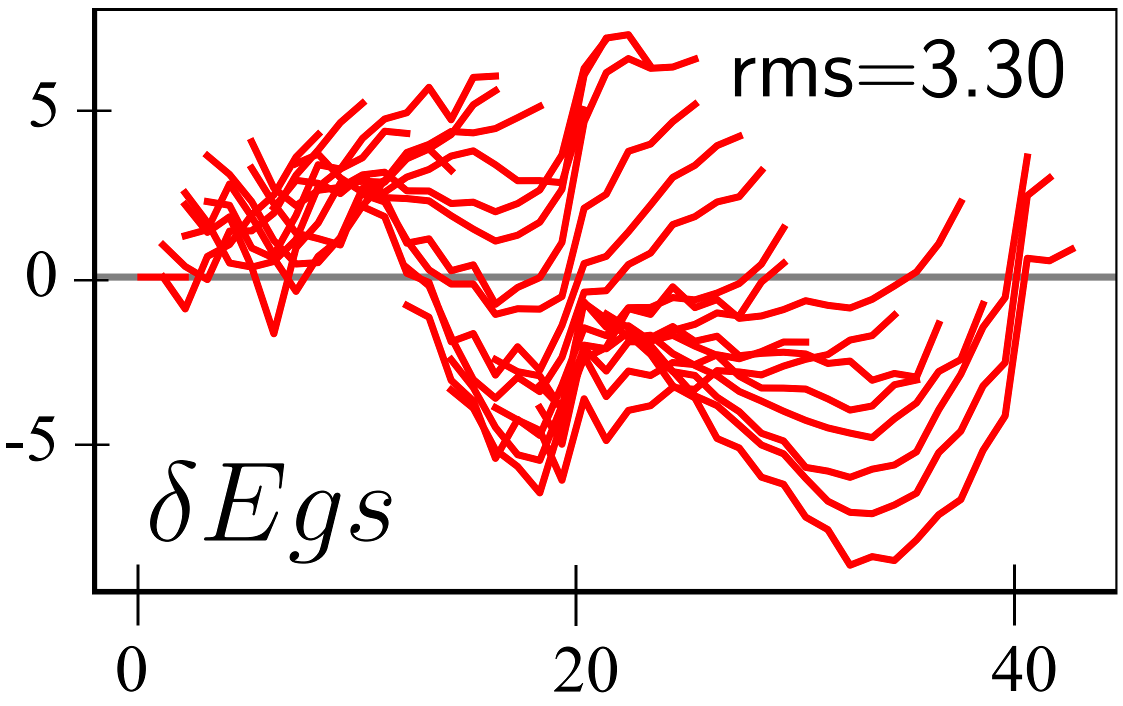
Phys. Rev. Lett. **126**, 022501 – Published 12 January 2021

Physics See synopsis: Predicting the Limits of Atomic Nuclei

Ab Initio Goes Global!

Long considered the domain of DFT or shell model

Ab initio calculations of ~700 nuclei from He to Fe!



$$\delta\mathcal{O} \equiv \mathcal{O}^{(th)} - \mathcal{O}^{(exp)}$$

B-W Mass formula: ~3.5MeV (Z<28)

DFT: 0.6-2.0 MeV

Input Hamiltonians fit to A=2,3,4 – **not biased towards known data**

Apply to proton/neutron driplines separation energies?

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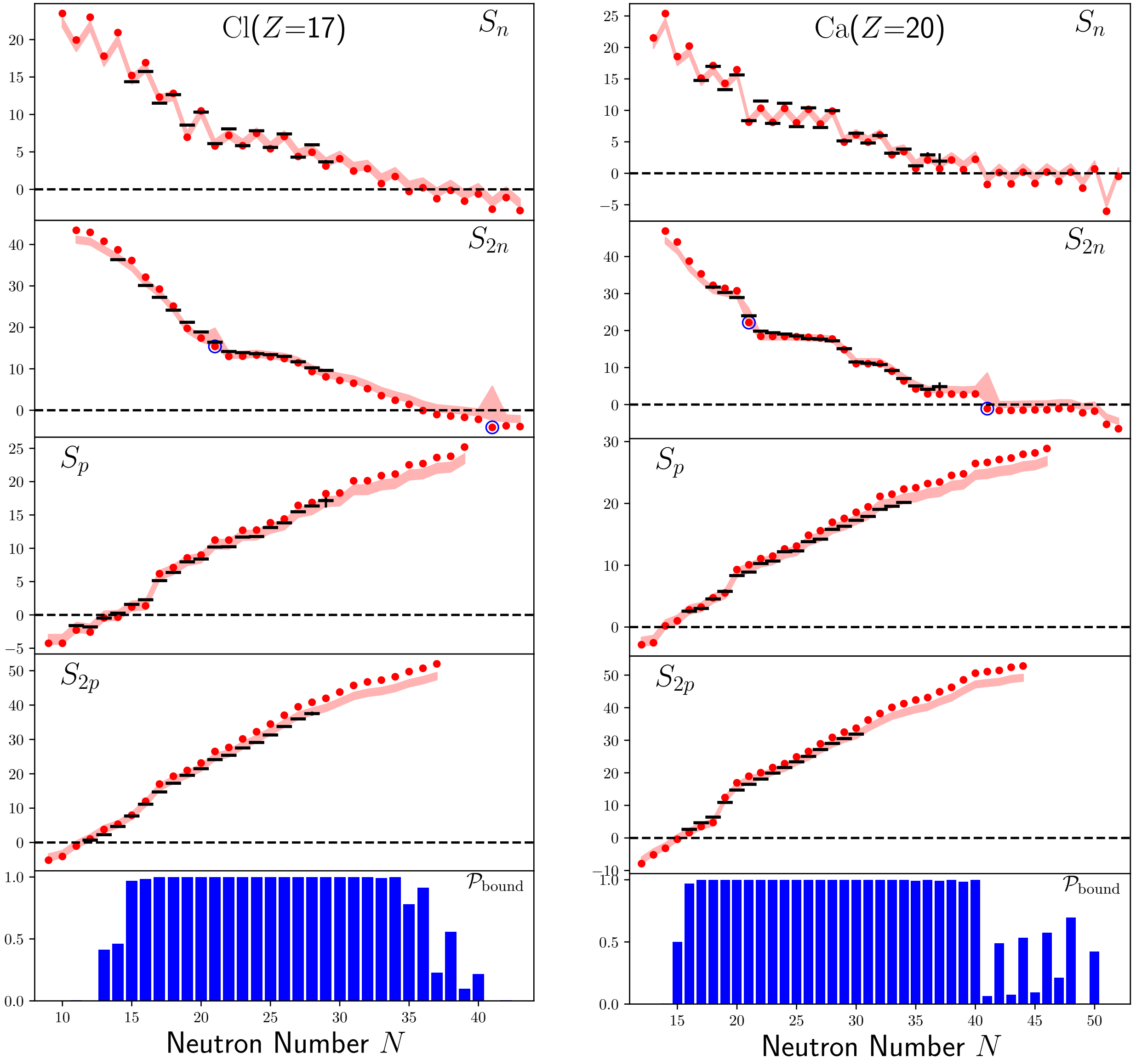
Estimating Separation Energy Uncertainties

rms deviation from experiment → model for theoretical uncertainties



rms = 0.7-1.4MeV

Obtain PPD for separation energies

$$p(\tilde{S}^{\mathrm{exp}}|\tilde{S}^{\mathrm{th}}, S^{\mathrm{th}}, S^{\mathrm{exp}})$$

Total probability to be bound

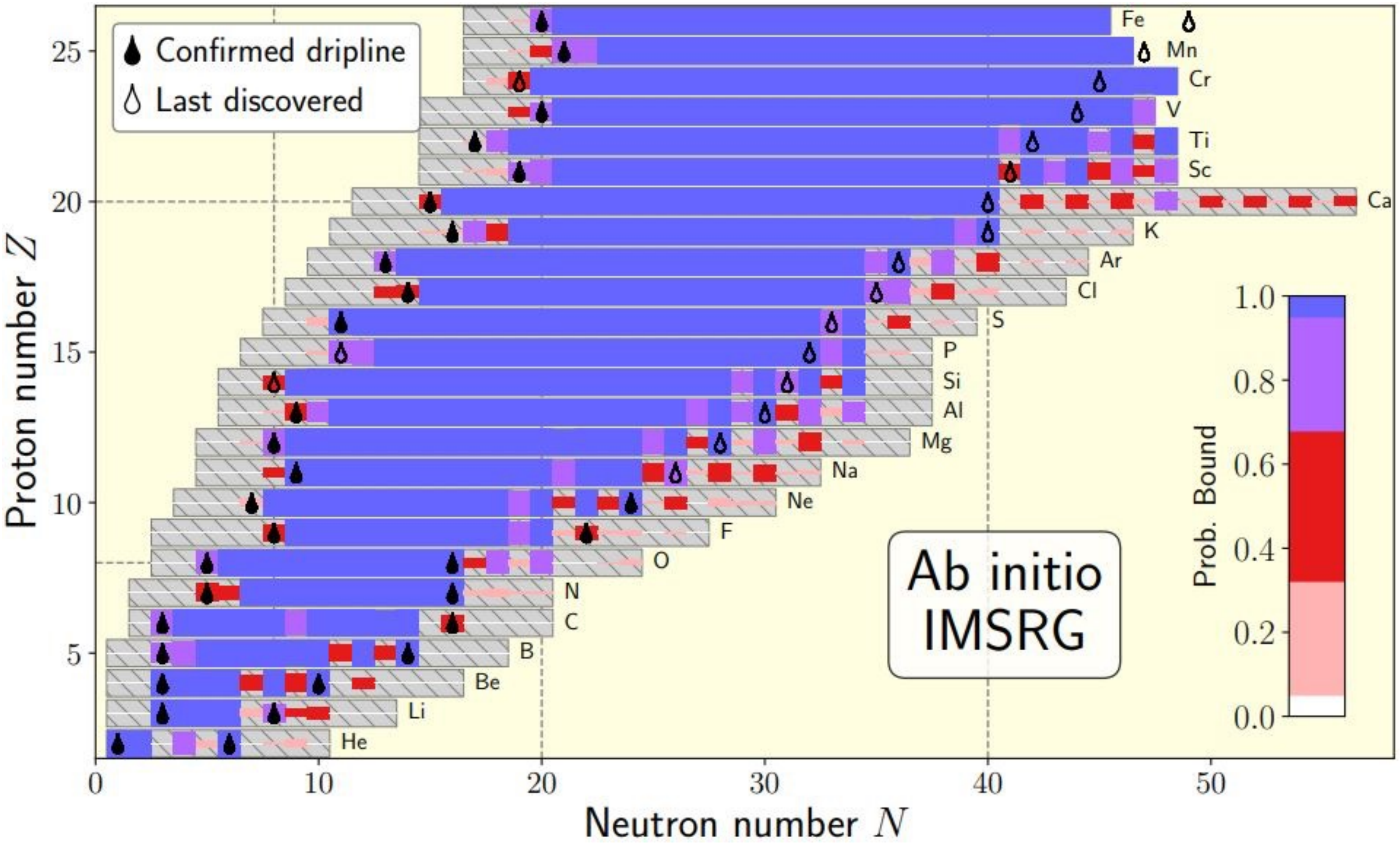
$$\mathcal{P}_{\mathrm{bound}} = \prod_{\alpha} \int_0^\infty d\tilde{S}_\alpha^{\mathrm{exp}} p(\tilde{S}_\alpha^{\mathrm{exp}}|\tilde{S}^{\mathrm{th}}, S^{\mathrm{th}}, S^{\mathrm{exp}})$$

$$\alpha \in \{n, p, 2n, 2p\}$$

Determine probabilities for each nucleus

Dripline Predictions to Medium Mass Region

Predictions of proton and neutron driplines from first principles



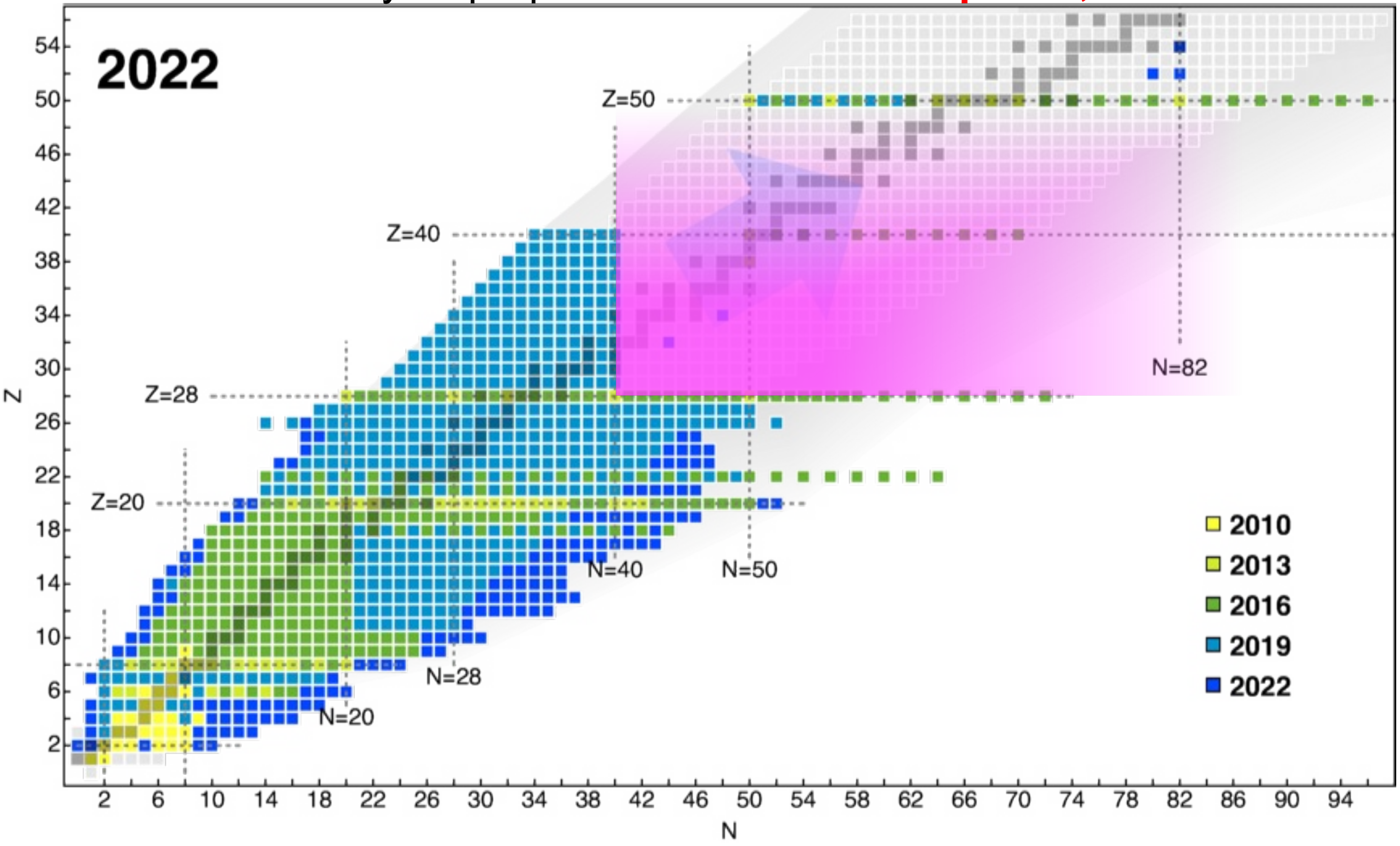
Known drip lines predicted within uncertainties (artifacts at shell closures)

Ab initio guide for neutron-rich driplines

Ab Initio Progress: How Heavy Can We Go?

Tremendous progress in ab initio reach, largely due to polynomially scaling methods!

Calculate essentially all properties all of nuclei… **up to N, Z ~ 50**



Key Limitation

3NF matrix element storage

$$e_1 + e_2 + e_3 \leq E_{3\max}$$

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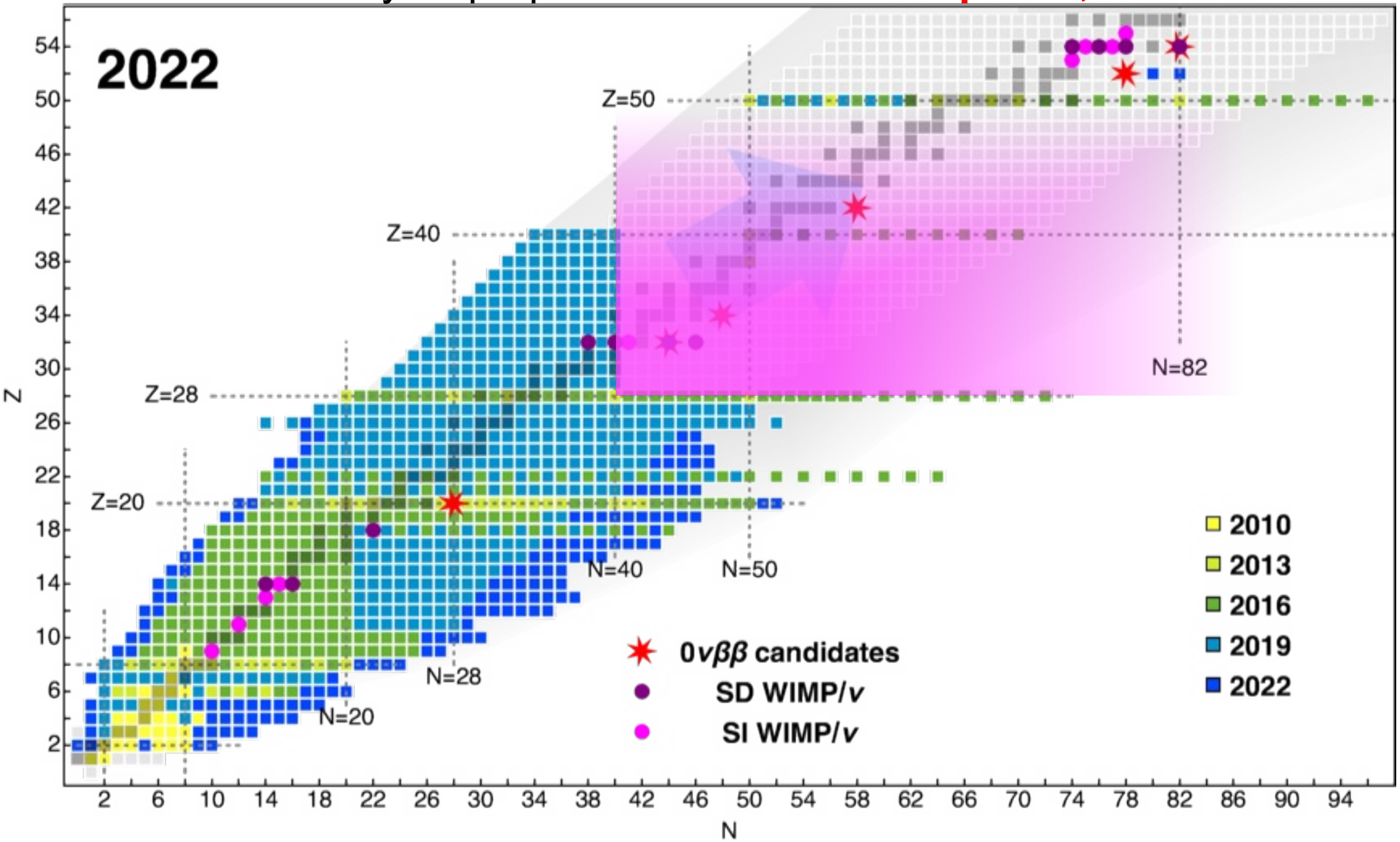

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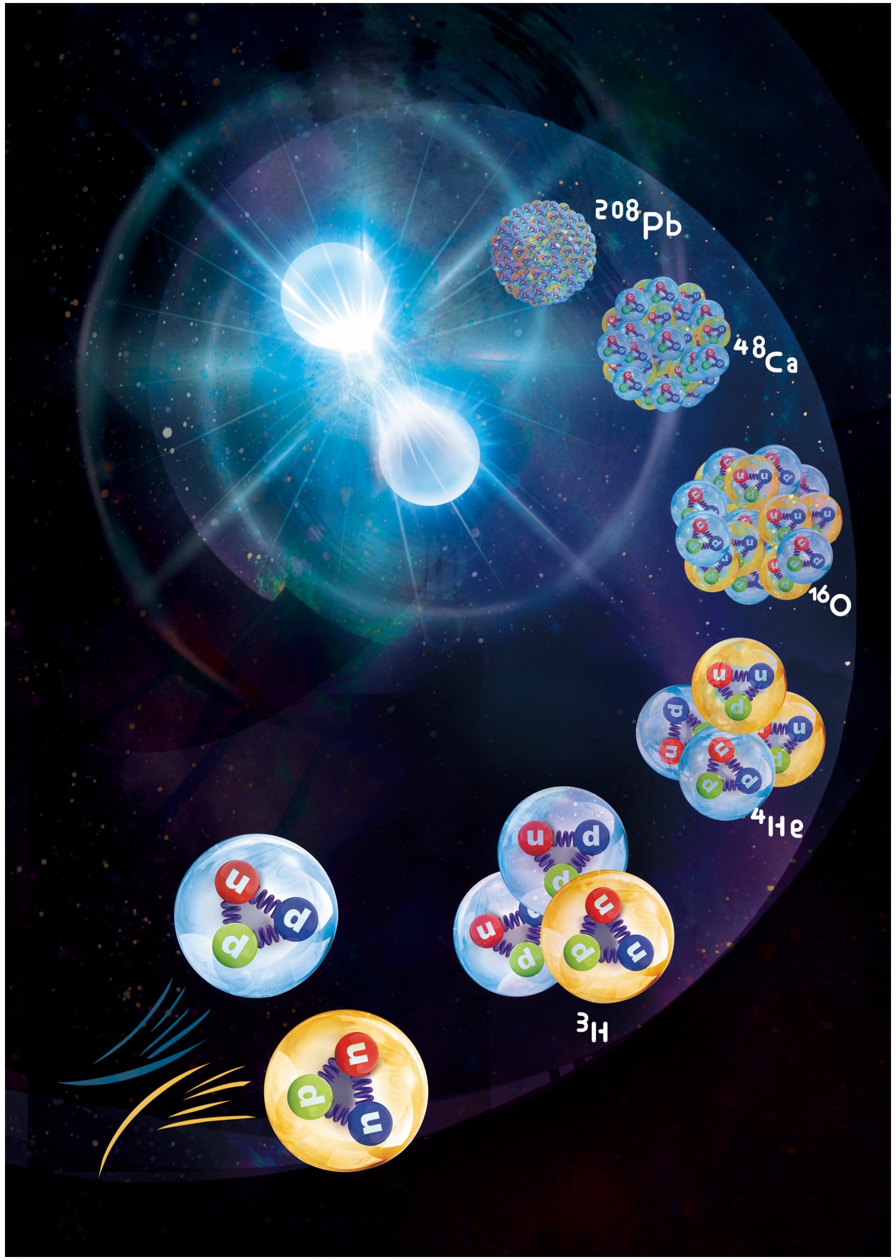
Converged Calculations in Heavy Nuclei



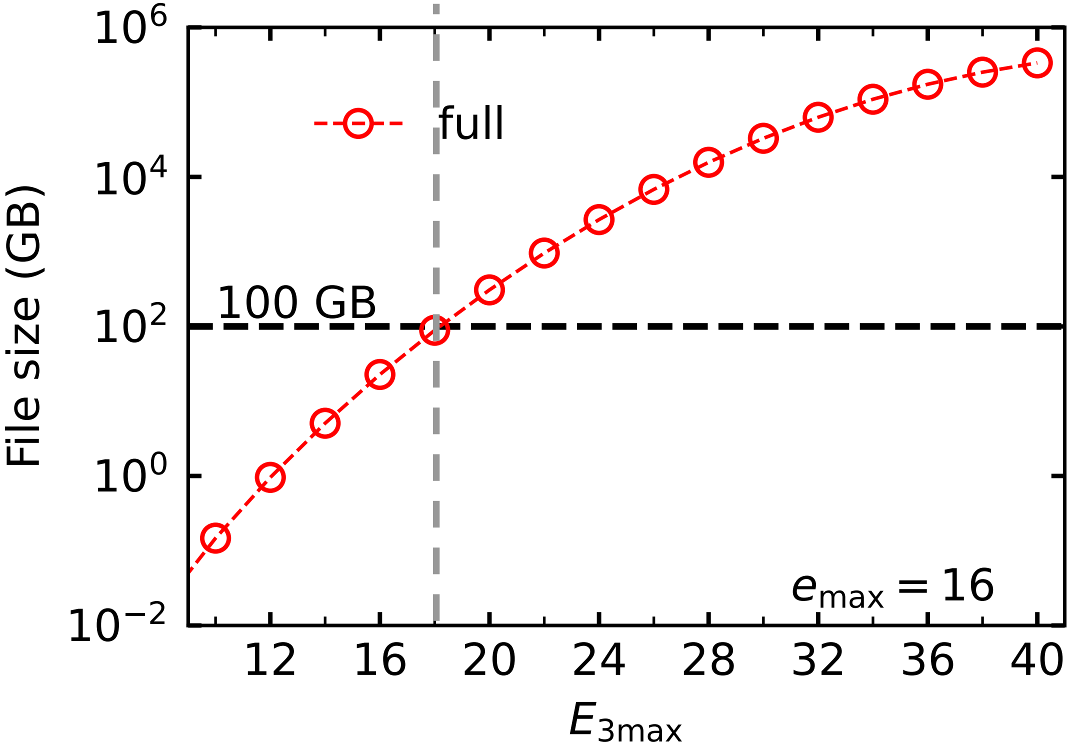
Converged *ab initio* calculations of heavy nuclei

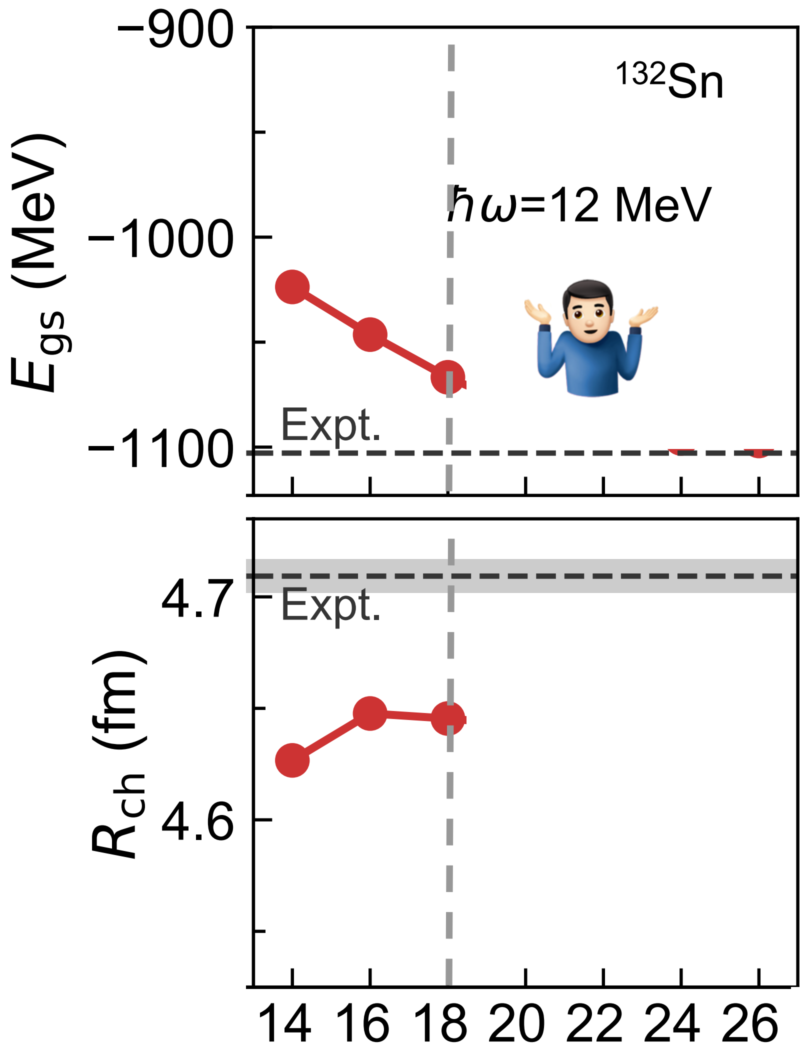
T. Miyagi, S. R. Stroberg, P. Navrátil, K. Hebeler, and J. D. Holt
Phys. Rev. C **105**, 014302 – Published 3 January 2022

Ab Initio Calculations of Heavy Nuclei

Limited by typical memory/node: $e_1 + e_2 + e_3 \leq E_{3\mathrm{max}} = 18$

No sign of convergence in ^{132}Sn - E_{gs} or R_{ch}

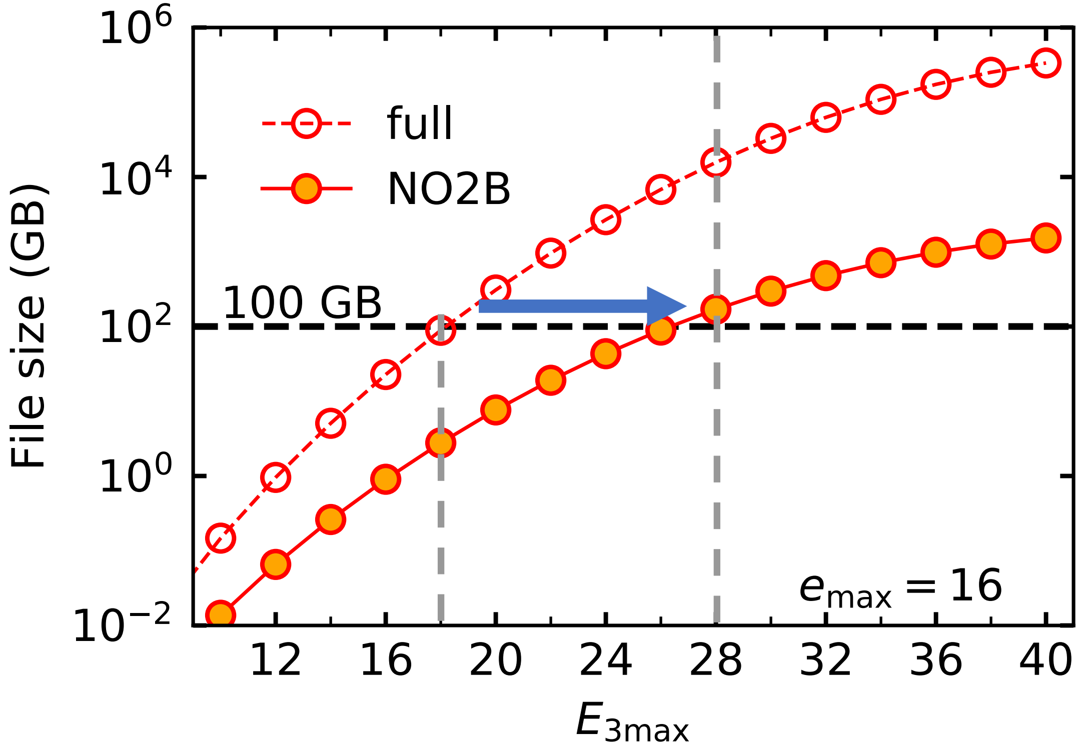


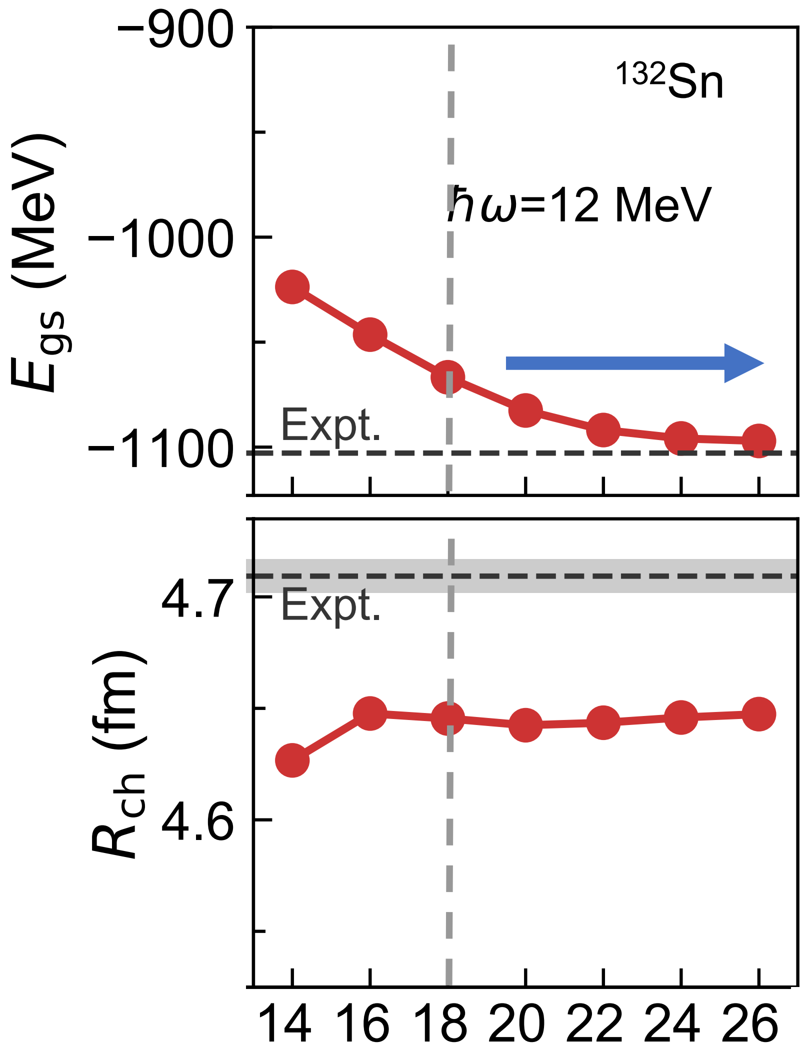


Ab Initio Calculations of Heavy Nuclei

Limited by typical memory/node: $e_1 + e_2 + e_3 \leq E_{3\mathrm{max}} = 18$

Clever storage reduces needs by factor of 100!





First converged ground-state properties of ^{132}Sn!

Opens heavy region to ab initio…

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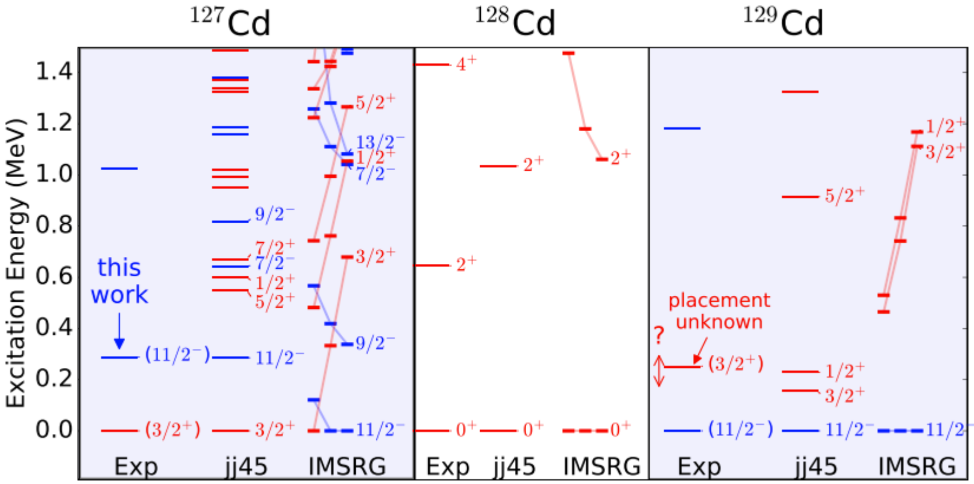
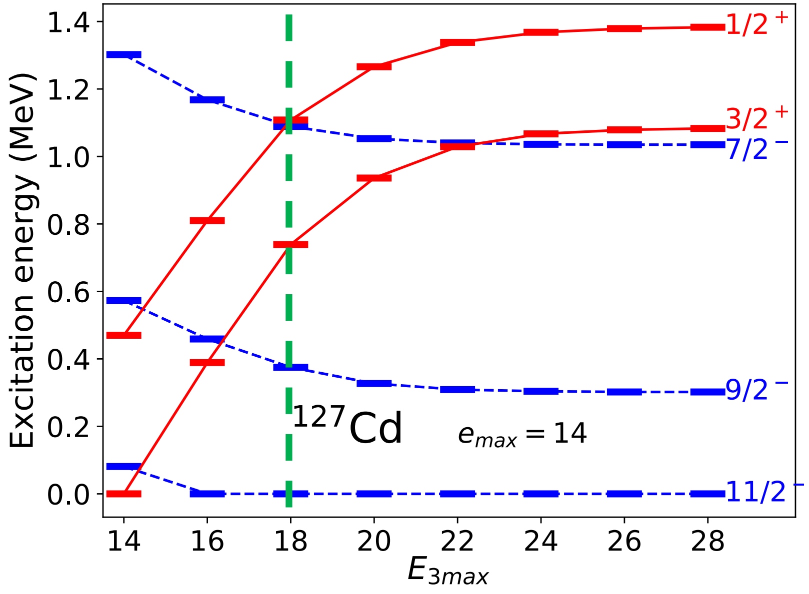
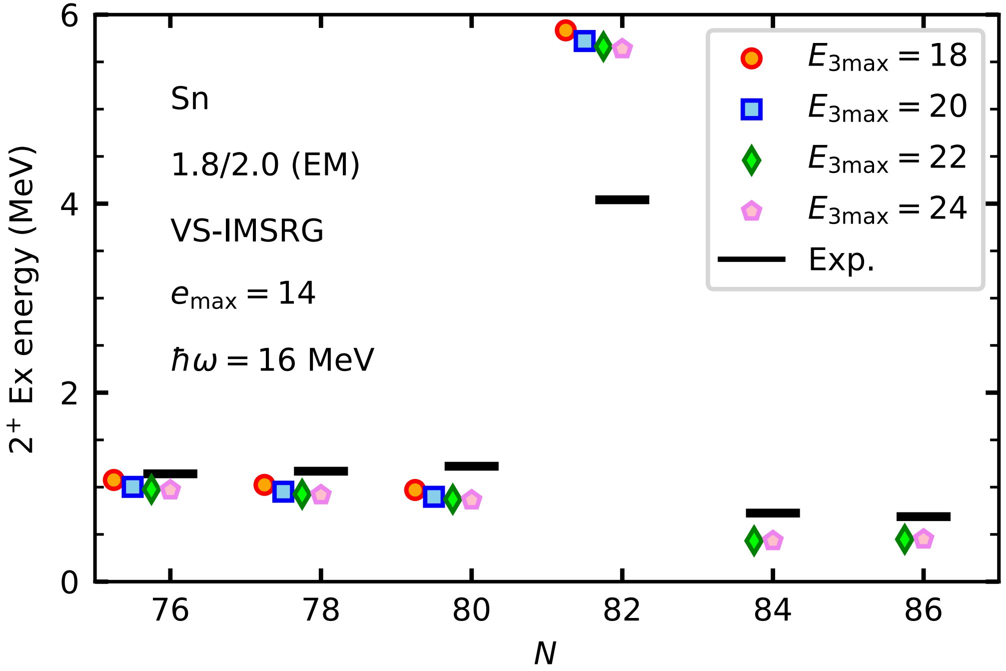
Convergence of N=82 Gap

Size of N=70 gap **well** converged at E_{3max}=28 for neutron-rich Sn, In, Cd!







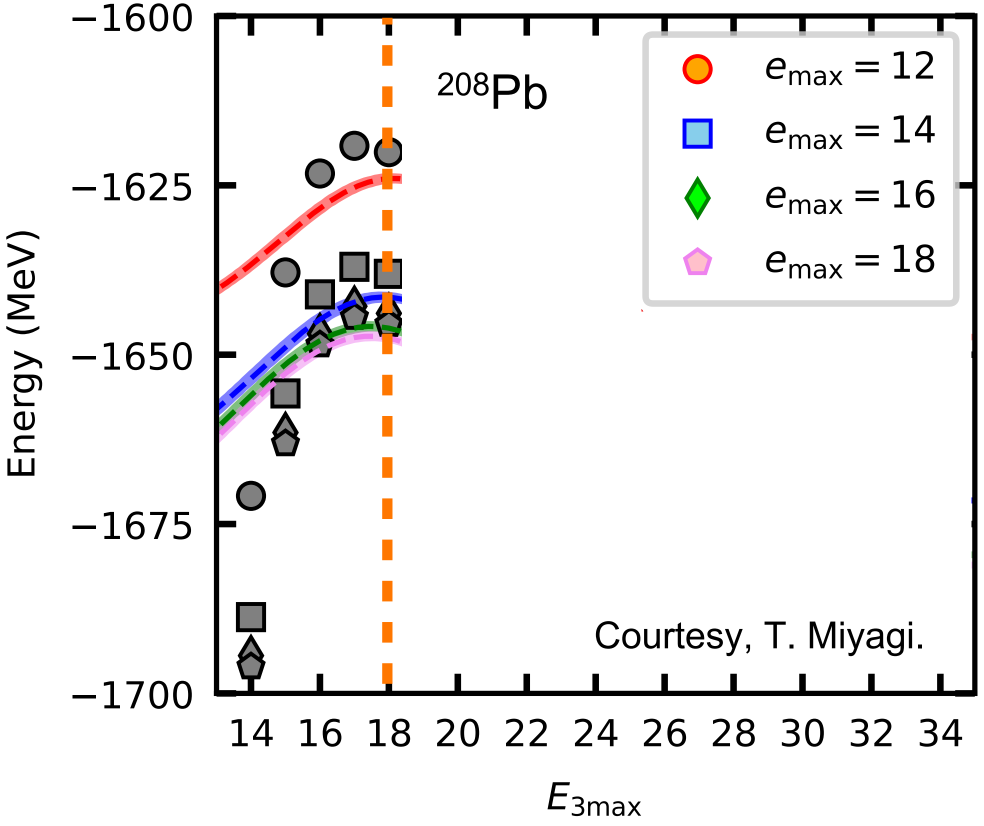
New capabilities: converged spectra in N=82 region

Converged (overpredicted) doubly magic ^{132}Sn

Can we go heavier?

Convergence in Heavy Nuclei: ^{208}Pb

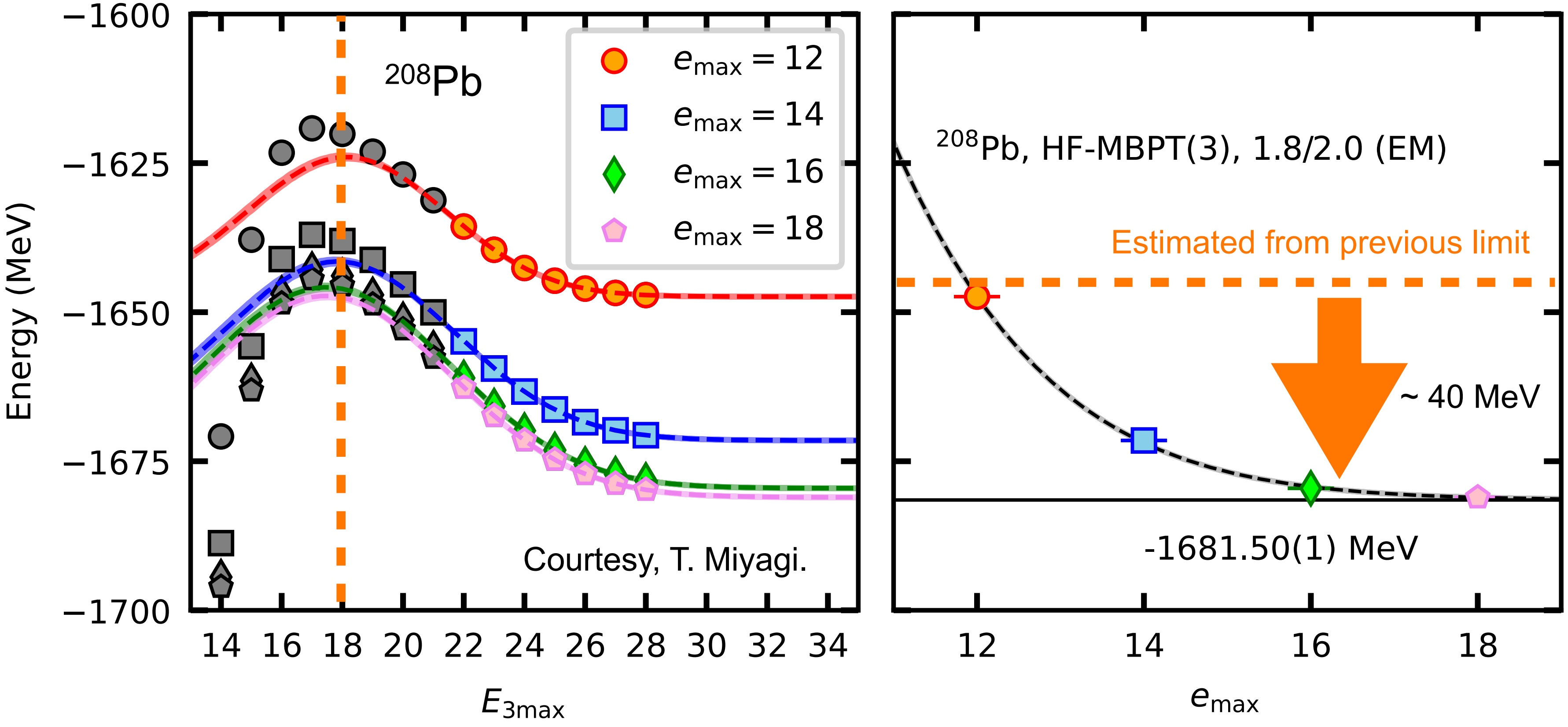
Previous limit, no hope of convergence in ^{208}Pb g.s. energy…



Convergence in Heavy Nuclei: ^{208}Pb

Previous limit, no hope of convergence in ^{208}Pb g.s. energy

Improved $E_{3\max} = 18 \rightarrow 28$ clear convergence



First converged ab initio calculation of ^{208}Pb!

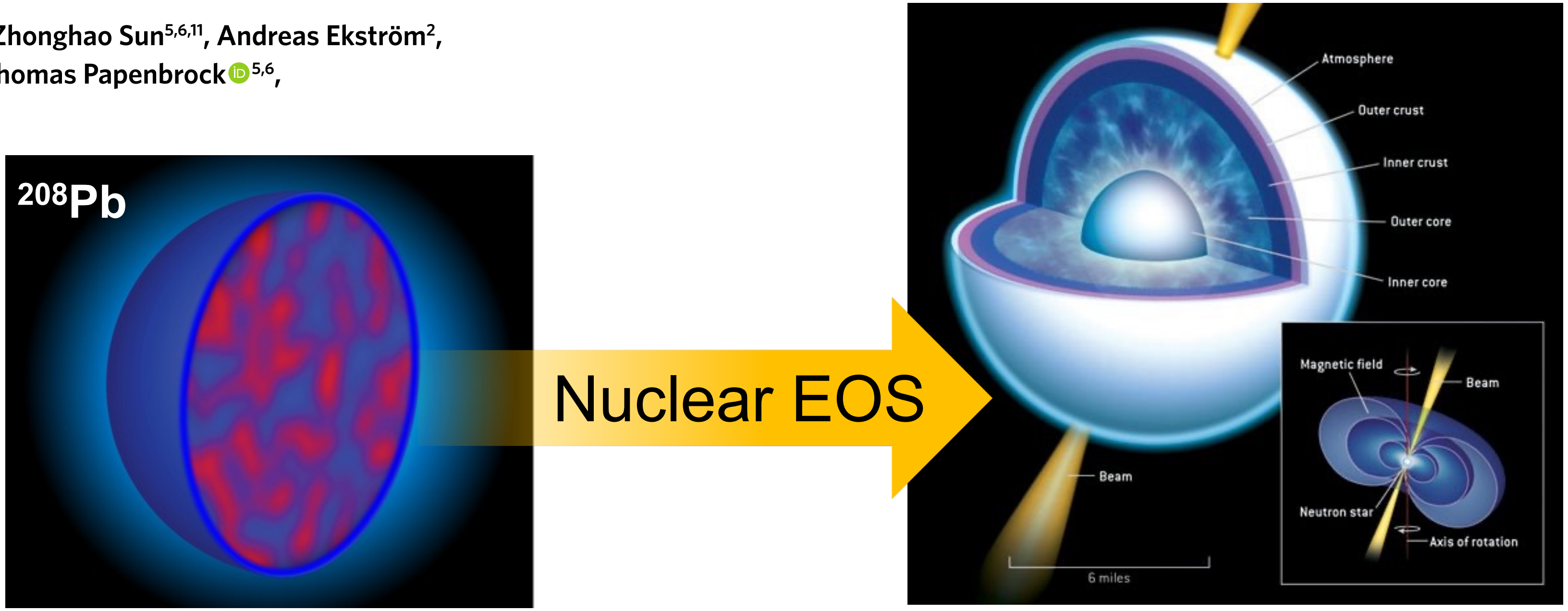
Ab Initio Analysis: Neutron Skin of ^{208}Pb Linked with neutron star properties

nature physics
ARTICLES
https://doi.org/10.1038/s41567-022-01715-8

OPEN

Ab initio predictions link the neutron skin of ^{208}Pb to nuclear forces

Baishan Hu[1,11], Weiguang Jiang[2,11], Takayuki Miyagi[1,3,4,11], Zhonghao Sun[5,6,11], Andreas Ekström[2], Christian Forssén[2] ✉, Gaute Hagen[1,5,6], Jason D. Holt[1,7], Thomas Papenbrock[5,6], S. Ragnar Stroberg[8,9] and Ian Vernon[10]



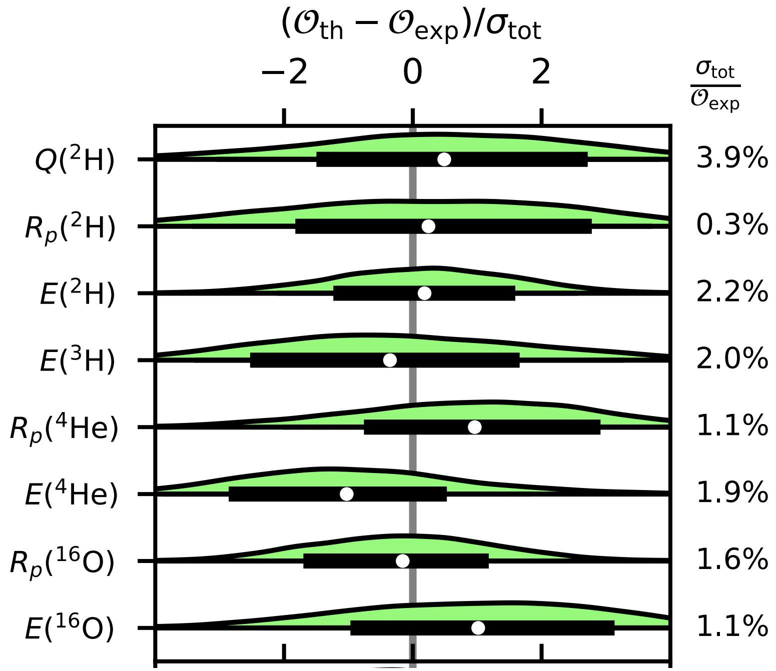
Neutron Skin of ^{208}Pb

Combine TRIUMF/ORNL/Chalmers advances!

I: History Matching confronted with A=2,3,4 data + ^{16}O

10^9 calculations spanning EFT parameter space at N^{2}LO

34 non-implausible interactions



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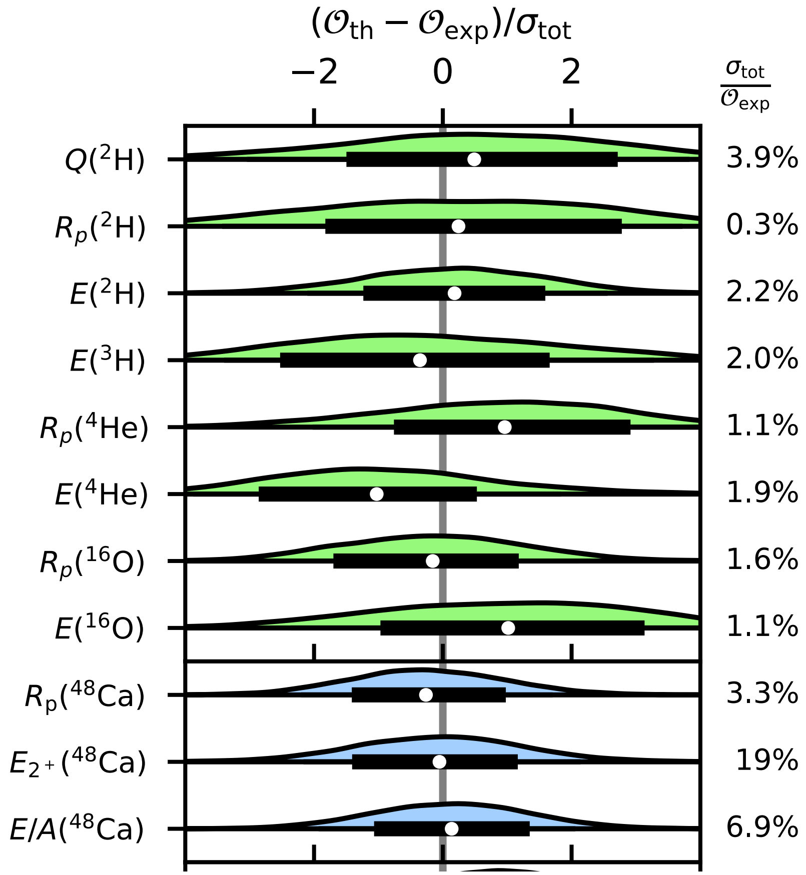
Importance resampling – statistically weight interactions



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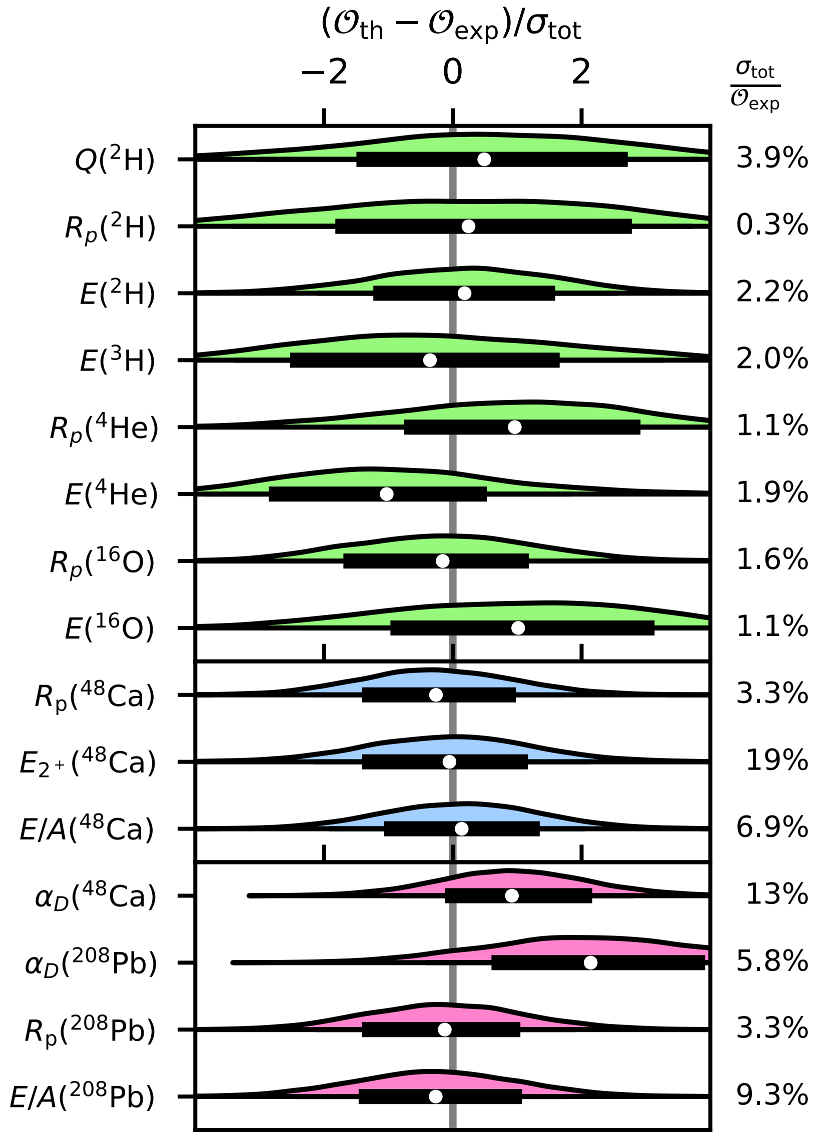
III: Validation ^{208}Pb E/A, R_p + ^{48}Ca/^{208}Pb DP from ab initio

Clear quality description of data



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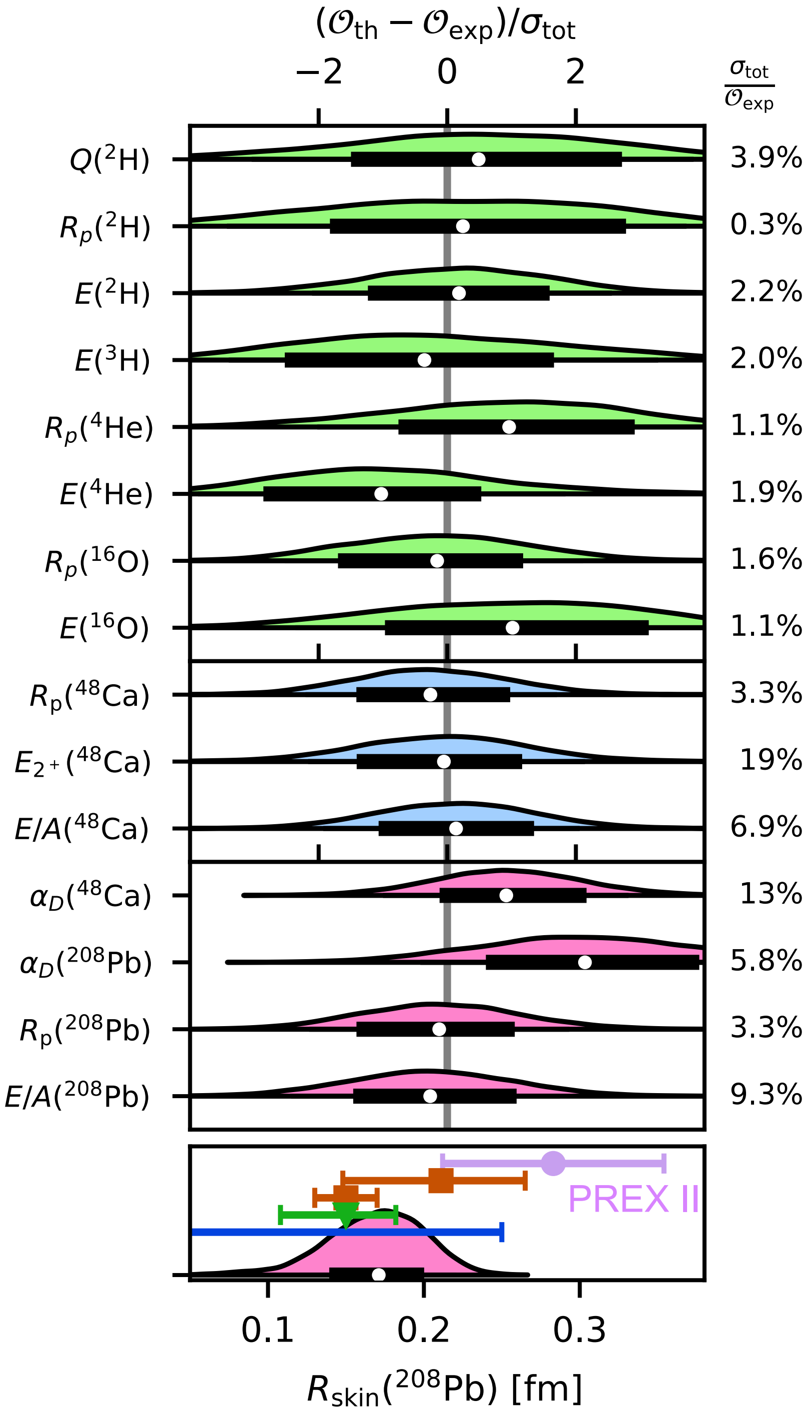
IV: Prediction - posterior predictive distribution for neutron skin

$R_{skin}(^{208}Pb)$= 0.14-0.20fm (68% credible level)

Consistent(ish) with extracted **PREXII result**



Infinite Matter Equation of State

Explore correlations between finite nuclei and nuclear EOS

Use same 34 non-implausible interactions

Reveals correlation as seen in mean field models

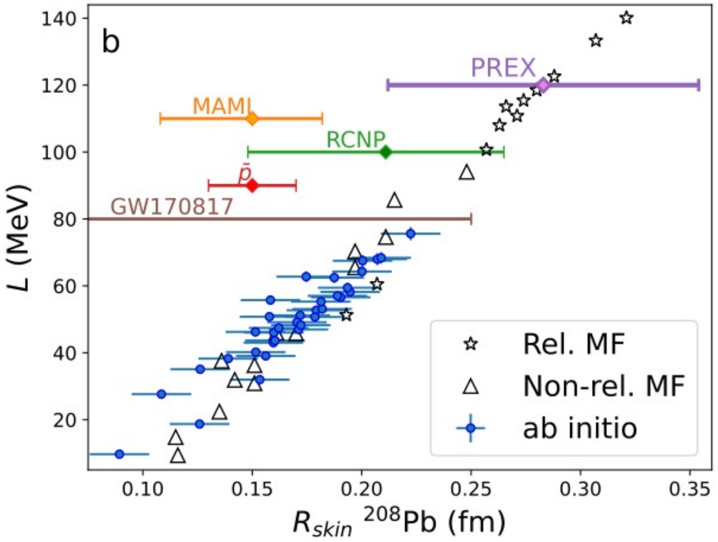
L = 37-63 MeV

Constrain forces potentially from:

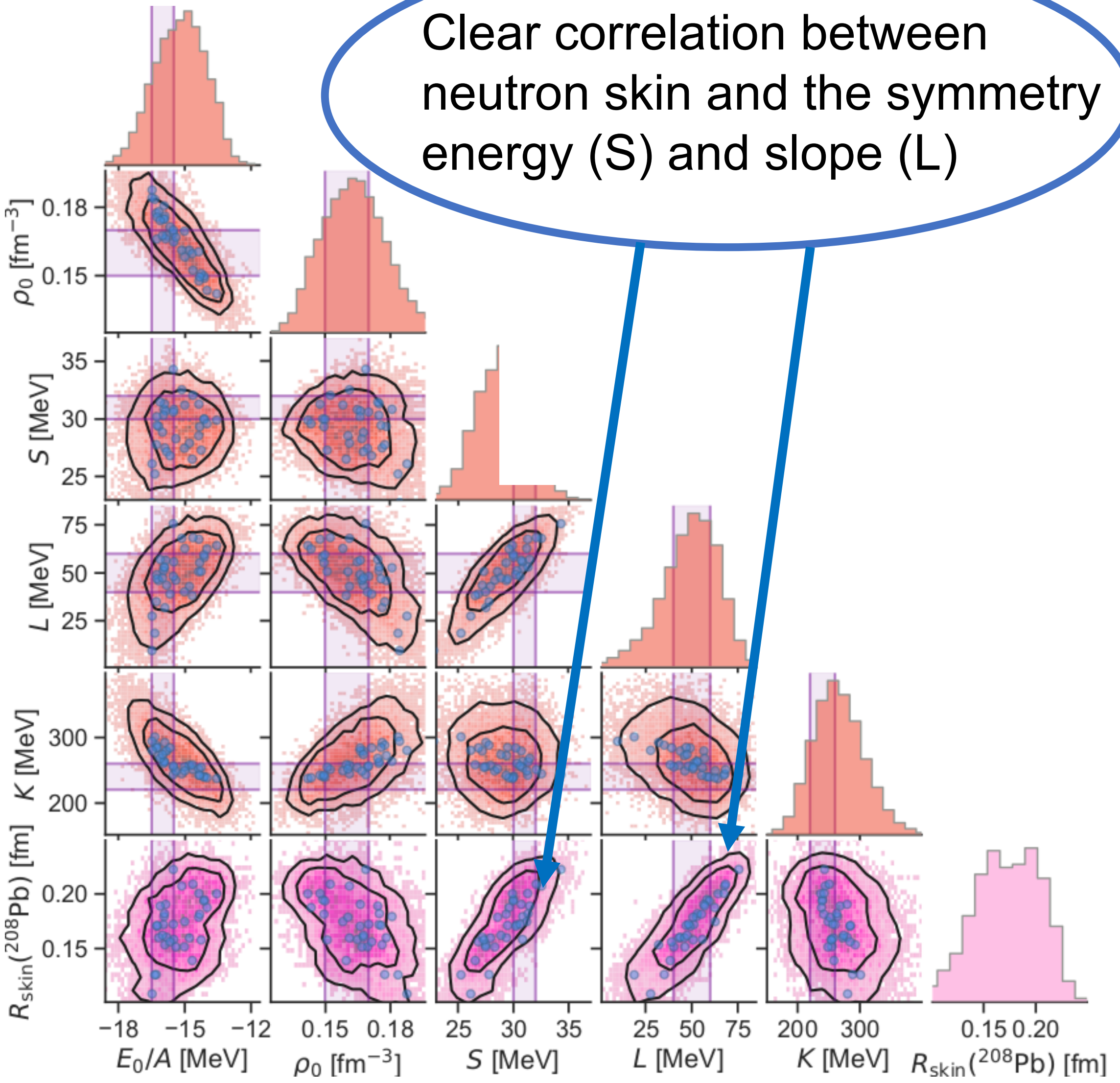
Neutron star radii/mergers

Mean field accommodates large range of skins

Tighter range from ab initio calculations

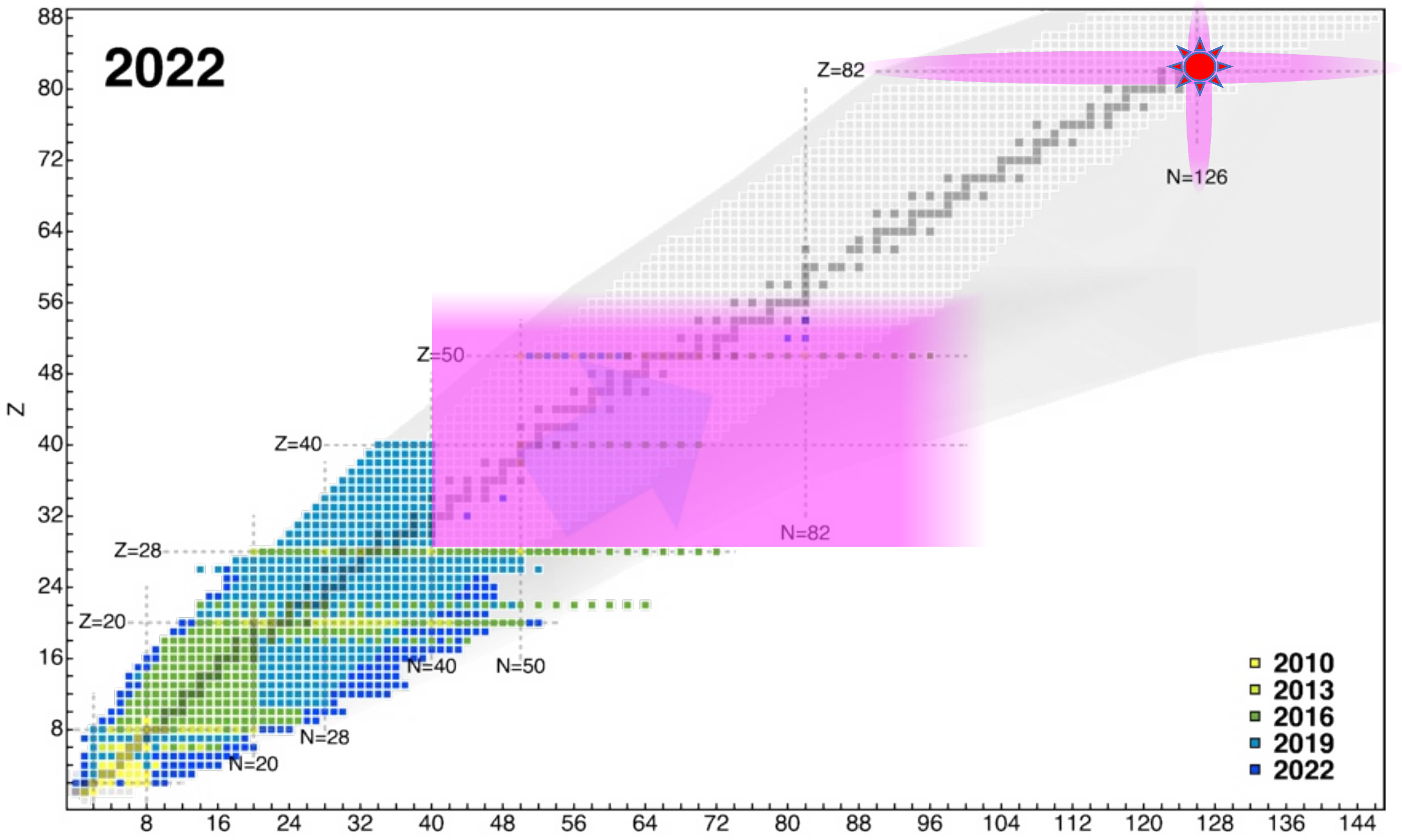


Clear correlation between neutron skin and the symmetry energy (S) and slope (L)



Recalibrating Ab Initio Progress

Rapid progress in ab initio reach, due to valence-space approach… up to...



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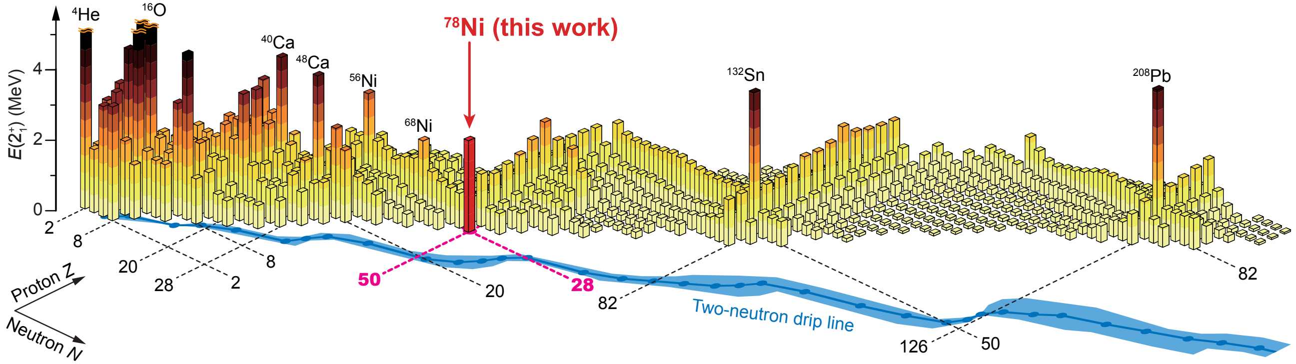
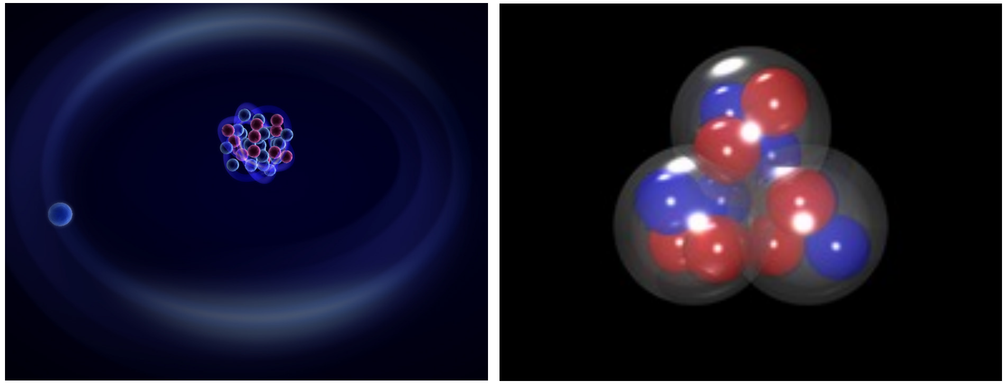
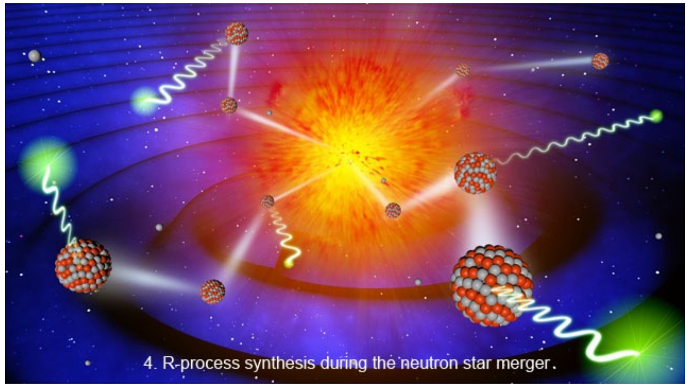
Major Questions in Nuclear Structure



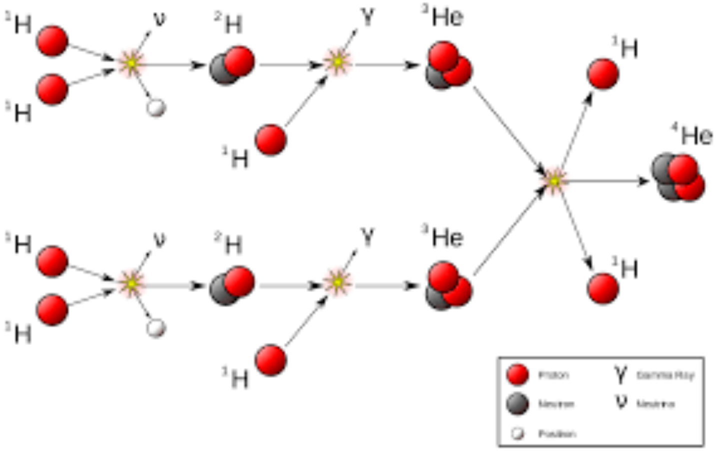


Limits of existence + formation/evolution of magic numbers

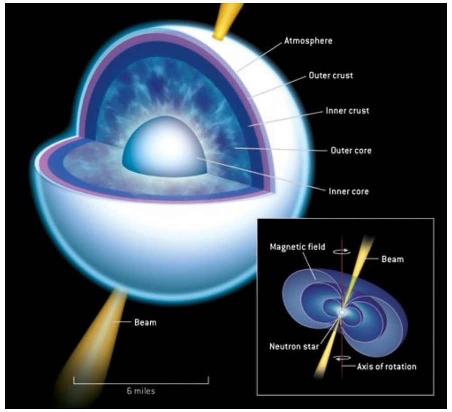
Nuclear radii/skins/halos/clusters



Heavy Nuclei + r-process



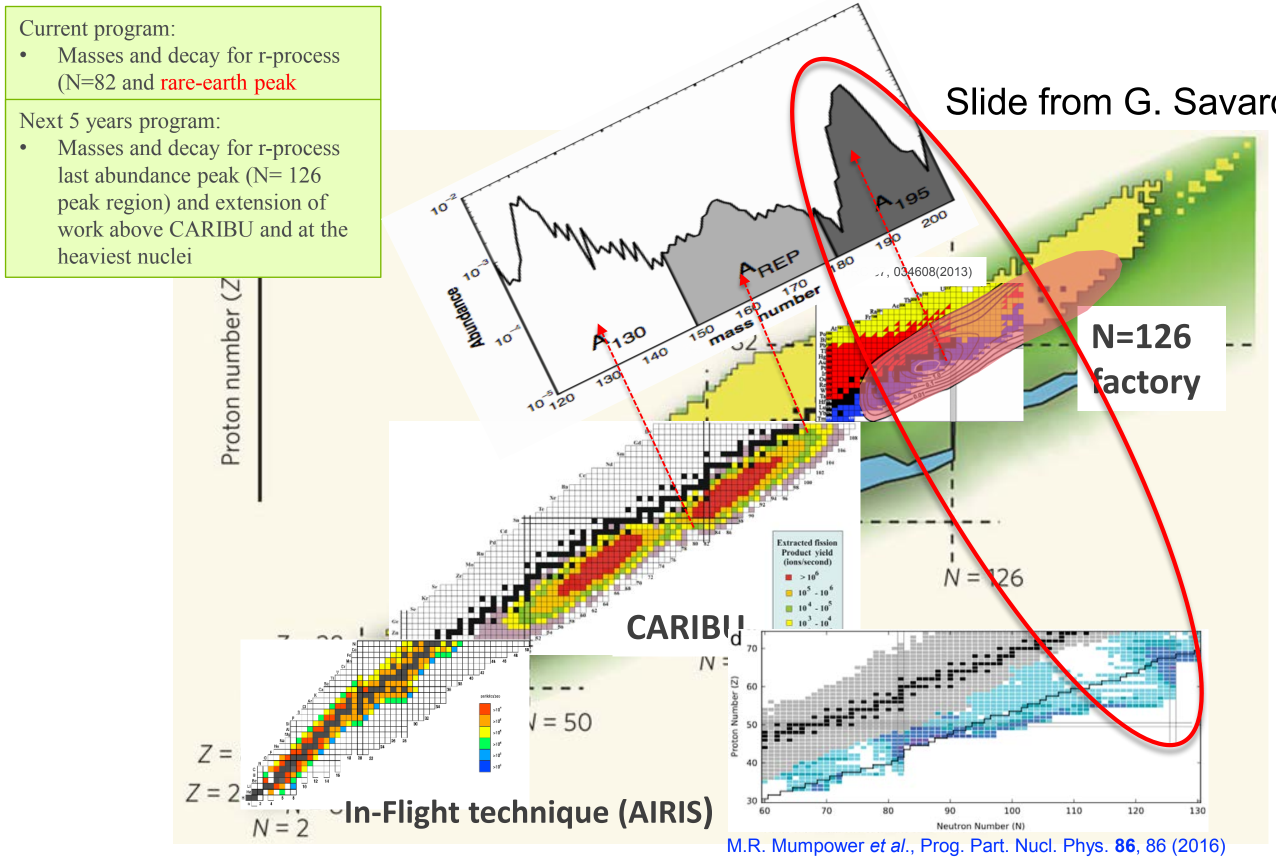
Continuum and nuclear reactions



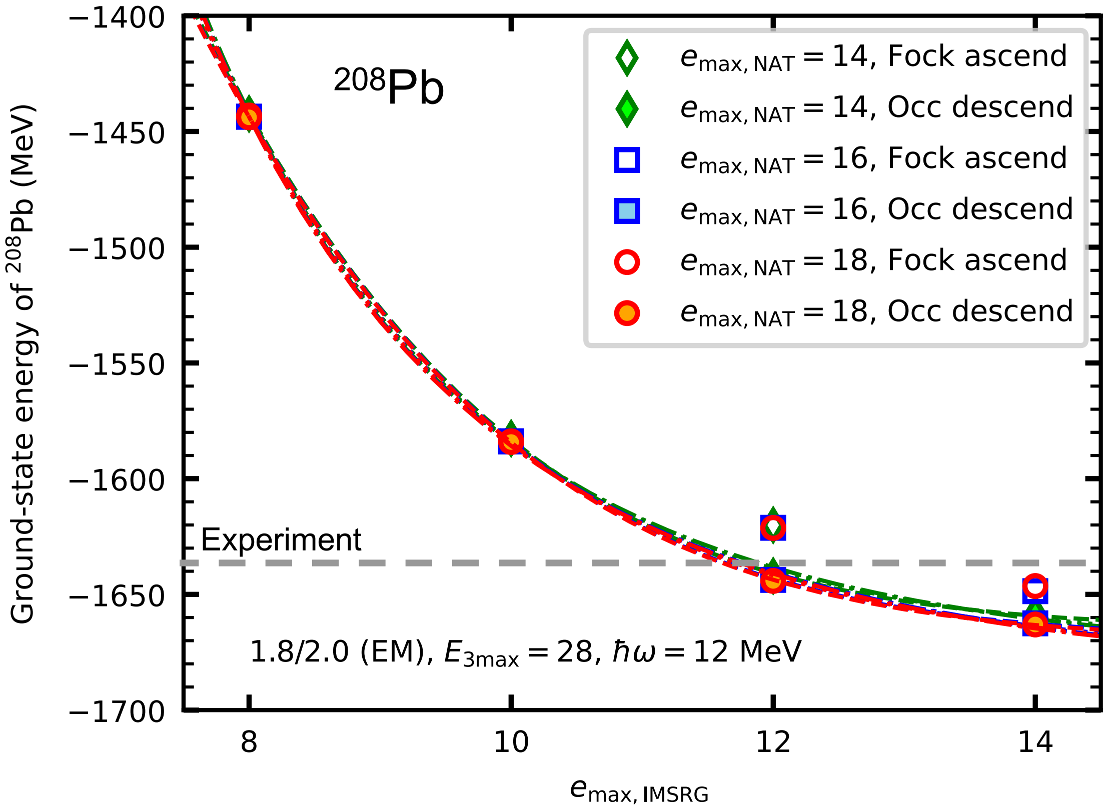
Infinite matter/Neutron stars

Ab Initio Theory for r-process

Information for nuclei along N=126 necessary for third r-process abundance peak



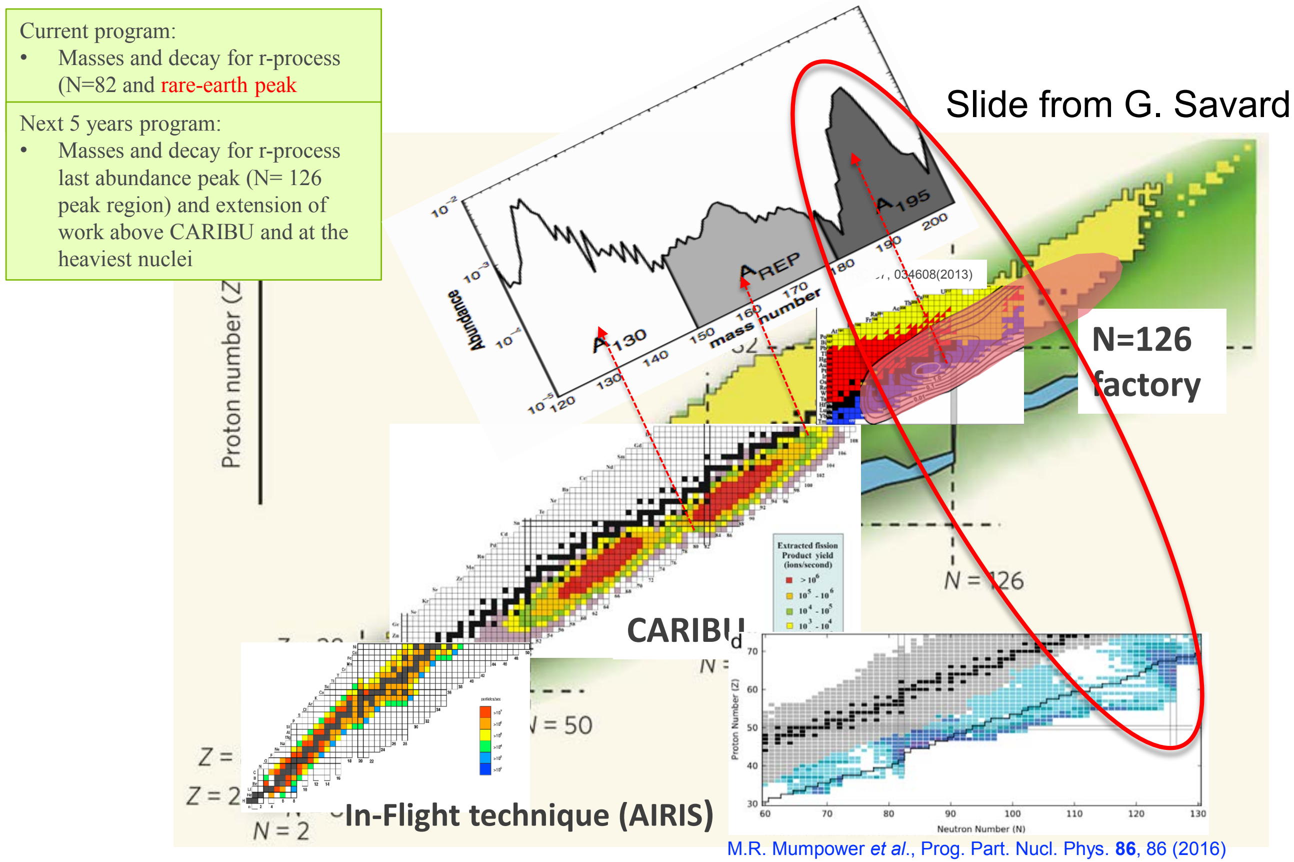
M.R. Mumpower *et al.*, Prog. Part. Nucl. Phys. **86**, 86 (2016)



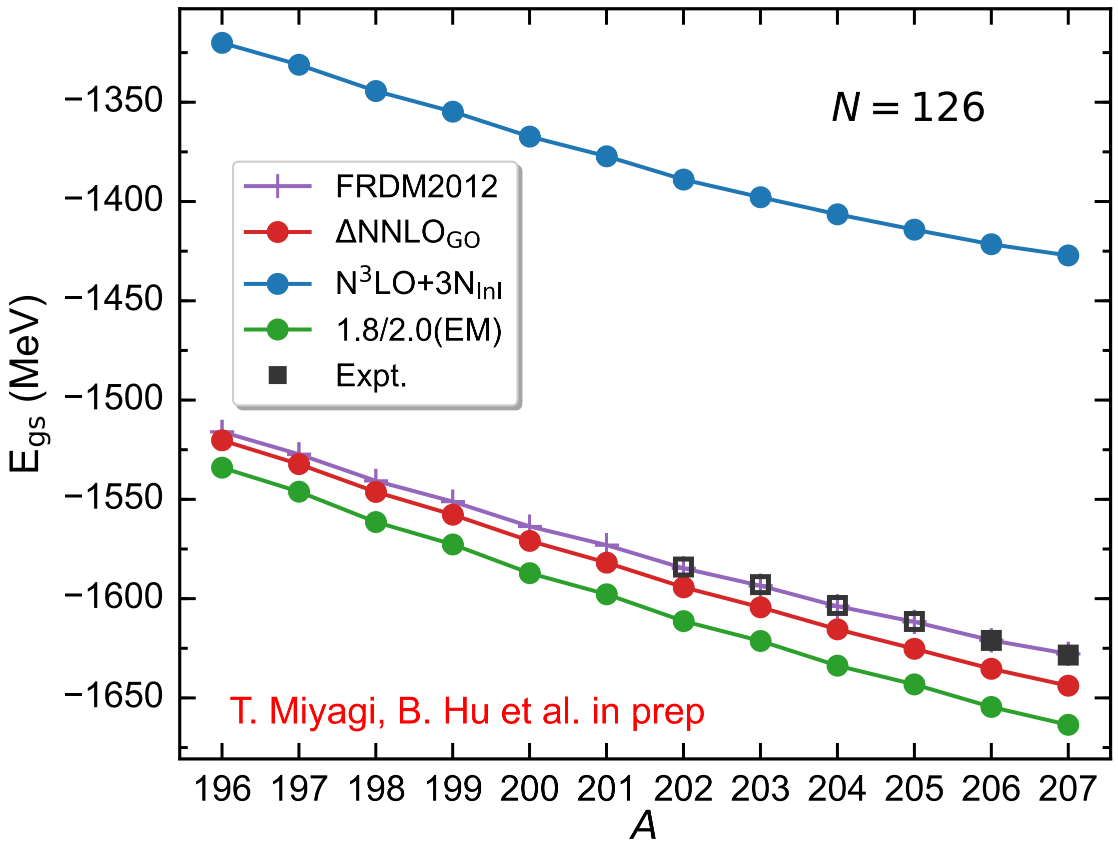
Natural Orbital Basis (NAT) allows for rapid convergence

Ab Initio Theory for r-process

Information for nuclei along N=126 necessary for third r-process abundance peak



M.R. Mumpower *et al.*, Prog. Part. Nucl. Phys. **86**, 86 (2016)



Natural Orbital Basis (NAT) allows for rapid convergence

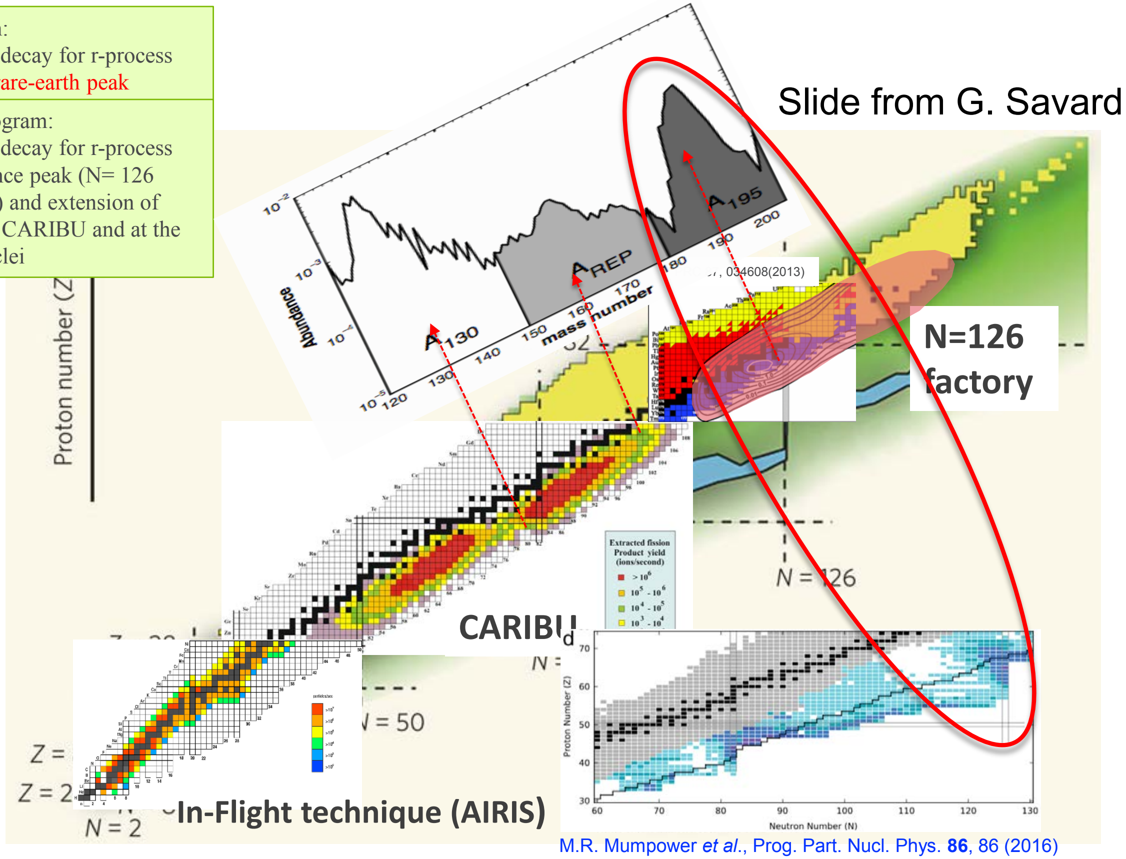
Converged ground-state energies for Z=69-82

Ab Initio Theory for r-process

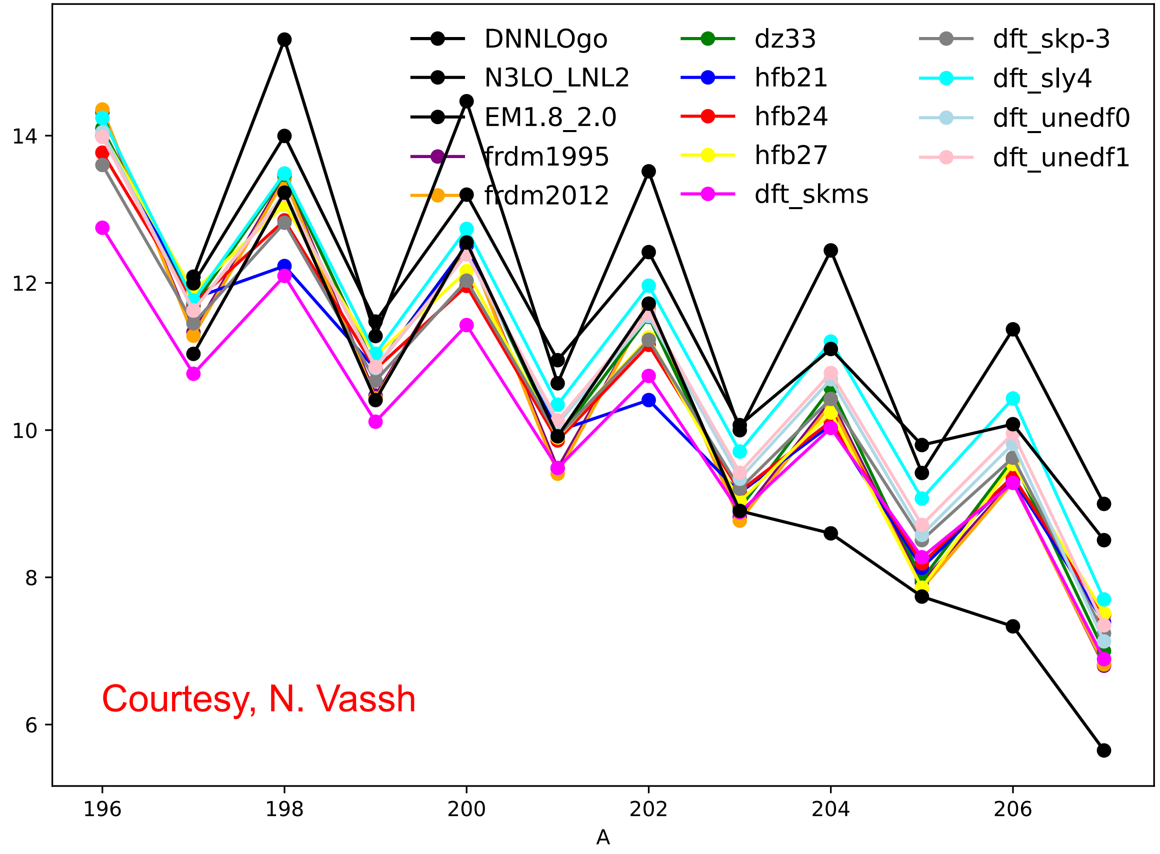
Information for nuclei along N=126 necessary for third r-process abundance peak

Current program:
- Masses and decay for r-process (N=82 and rare-earth peak

Next 5 years program:
- Masses and decay for r-process last abundance peak (N= 126 peak region) and extension of work above CARIBU and at the heaviest nuclei



M.R. Mumpower *et al.*, Prog. Part. Nucl. Phys. **86**, 86 (2016)

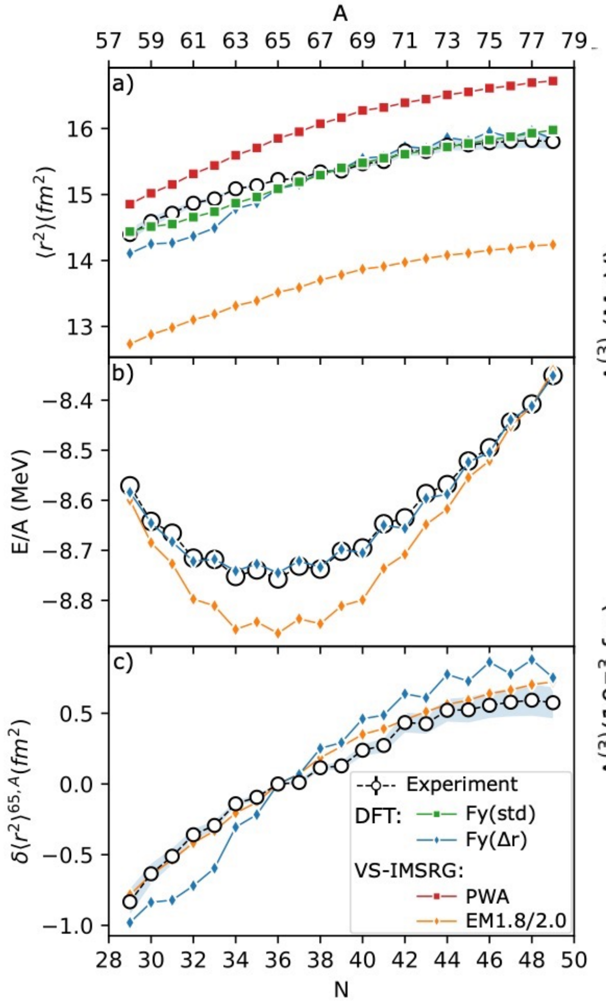


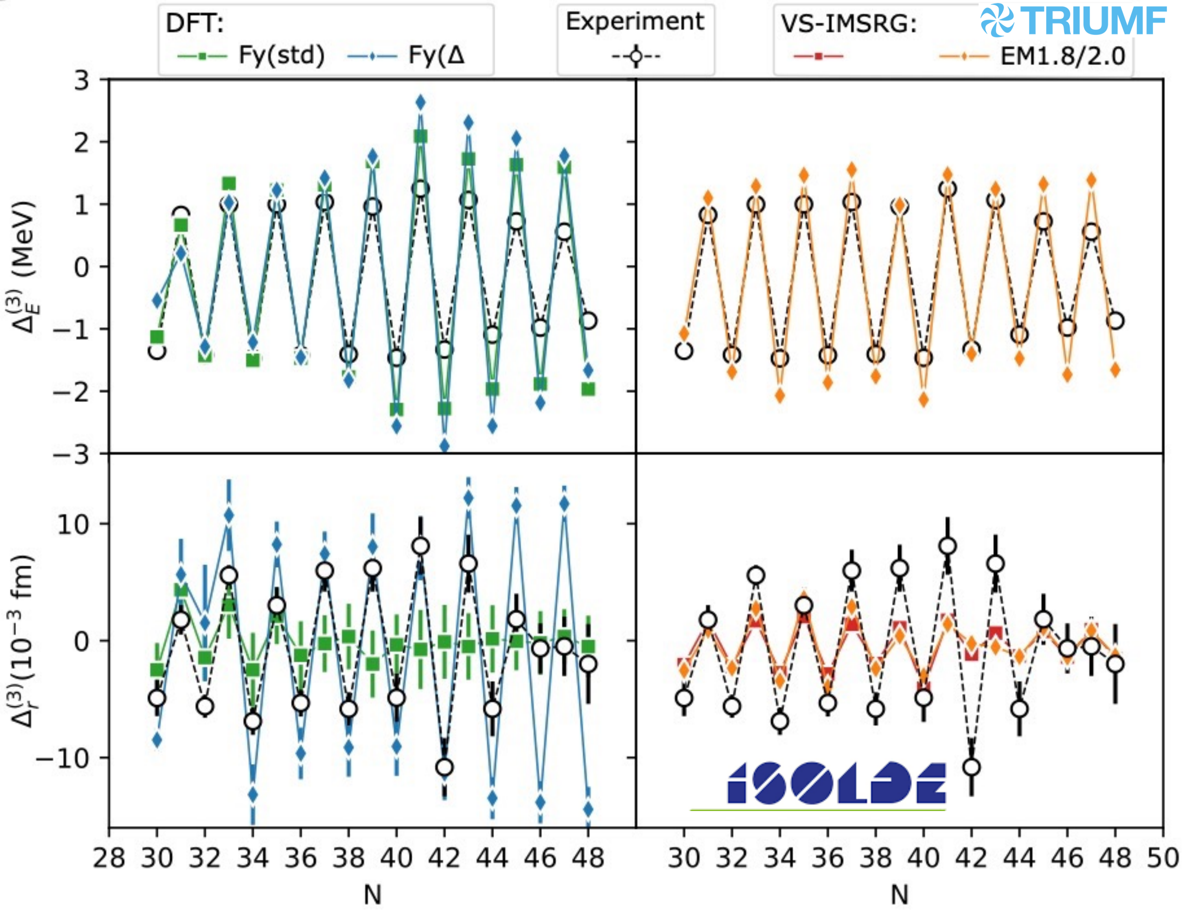
Natural Orbital Basis (NAT) allows for rapid convergence

Significant systematic differences from mass models for S_p

TRIUMF Laser Spectroscopy: Charge Radii of Cu Isotopes

Odd-even staggering of charge radii across Cu chain





LETTERS

https://doi.org/10.1038/s41567-020-0868-y

nature physics

Check for updates

OPEN

Measurement and microscopic description of odd–even staggering of charge radii of exotic copper isotopes

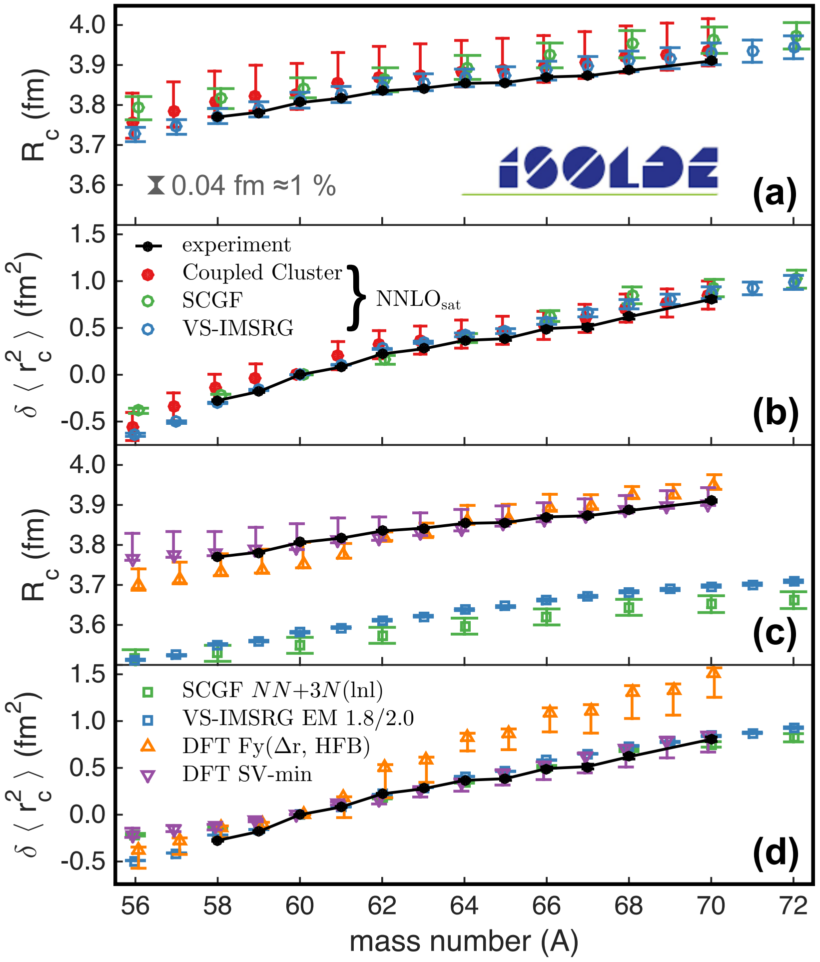
R. P. de Groote[1,2], J. Billowes[3], C. L. Binnersley[3], M. L. Bissell[3], T. E. Cocolios[1], T. Day Goodacre[4,5], G. J. Farooq-Smith[1], D. V. Fedorov[6], K. T. Flanagan[3], S. Franchoo[7], R. F. Garcia Ruiz[3,8,9], W. Gins[1,2], J. D. Holt[5,10], Á. Koszorús[1], K. M. Lynch[9], T. Miyagi[5], W. Nazarewicz[11], G. Neyens[1,9], P.-G. Reinhard[12], S. Rothe[3,4], H. H. Stroke[13], A. R. Vernon[1,3], K. D. A. Wendt[14], S. G. Wilkins[3,4], Z. Y. Xu[1] and X. F. Yang[1,15]

Cu isotopes, odd-even staggering well reproduced

Ab initio competitive with DFT (fit to reproduce odd-even staggering)

Laser Spectroscopy: Charge Radii of Ni Isotopes

Study charge radii systematics across Ni isotopic chain



Nuclear Charge Radii of the Nickel Isotopes $^{58-68,70}$Ni

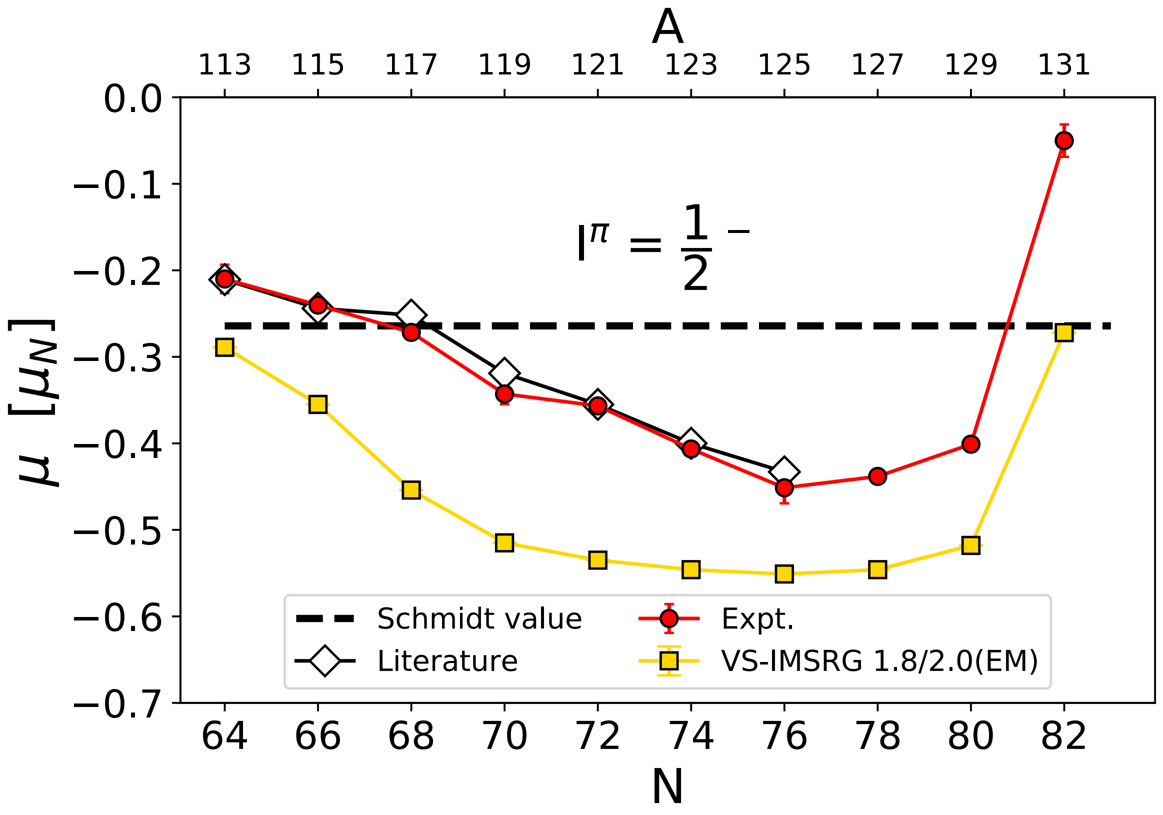
S. Malbrunot-Ettenauer *et al.*
Phys. Rev. Lett. **128**, 022502 – Published 14 January 2022

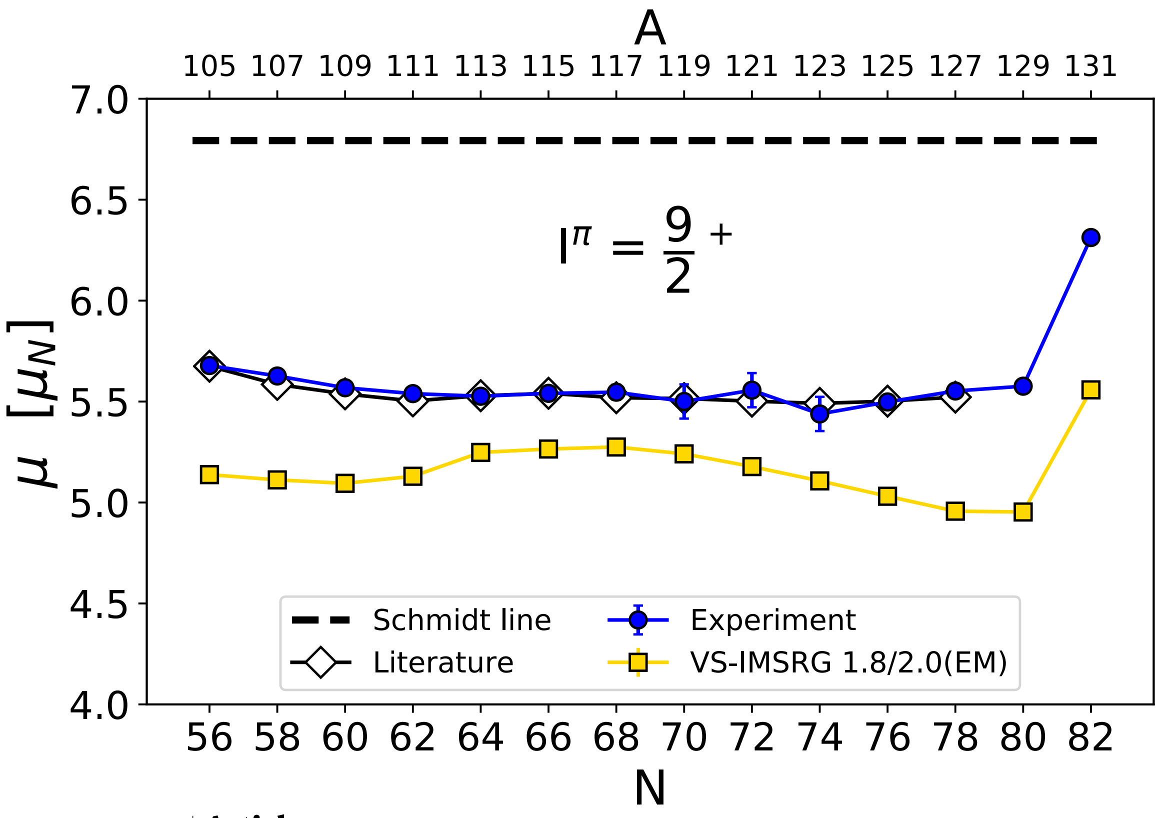
Multiple ab-initio methods largely agree within uncertainties

Ab initio (again) competitive/complementary with DFT

EM Moments in Neutron-Rich In Isotopes

Electromagnetic moments of entire In chain – sharp increase at N=82





Ab initio reproduces trends of new measurements

Neglected physics: two-body meson-exchange currents

Article

Nuclear moments of indium isotopes reveal abrupt change at magic number 82

https://doi.org/10.1038/s41586-022-04818-7

Received: 10 June 2021

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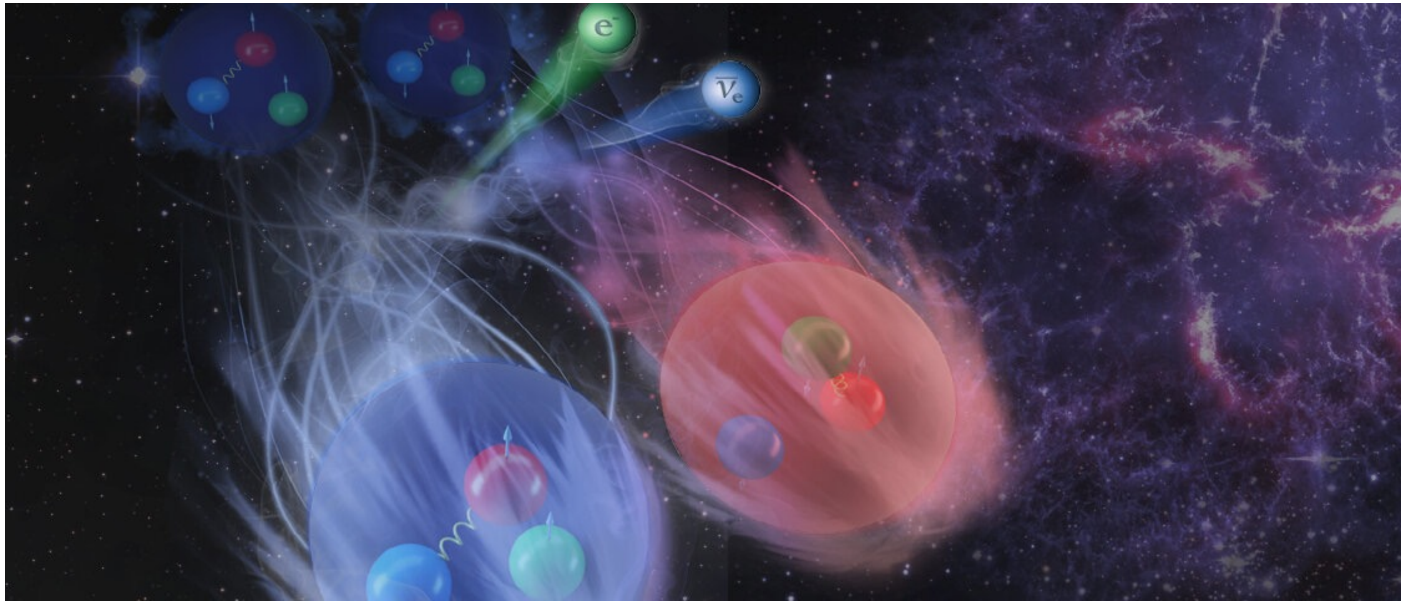
A. R. Vernon[1,2,3]✉, R. F. Garcia Ruiz[2,4]✉, T. Miyagi[5], C. L. Binnersley[1], J. Billowes[1], M. L. Bissell[1], J. Bonnard[6], T. E. Cocolios[3], J. Dobaczewski[6,7], G. J. Farooq-Smith[3], K. T. Flanagan[1,8], G. Georgiev[9], W. Gins[3,10], R. P. de Groote[3,10], R. Heinke[4,11], J. D. Holt[5,12], J. Hustings[3], Á. Koszorús[3], D. Leimbach[11,13,14], K. M. Lynch[4], G. Neyens[3,4], S. R. Stroberg[15], S. G. Wilkins[1,2], X. F. Yang[3,16] & D. T. Yordanov[4,9]

TRIUMF

Two-Body Currents for Gamow-Teller Transitions and g_A Quenching



LETTERS
https://doi.org/10.1038/s41567-019-0450-7
nature physics

Discrepancy between experimental and theoretical β-decay rates resolved from first principles

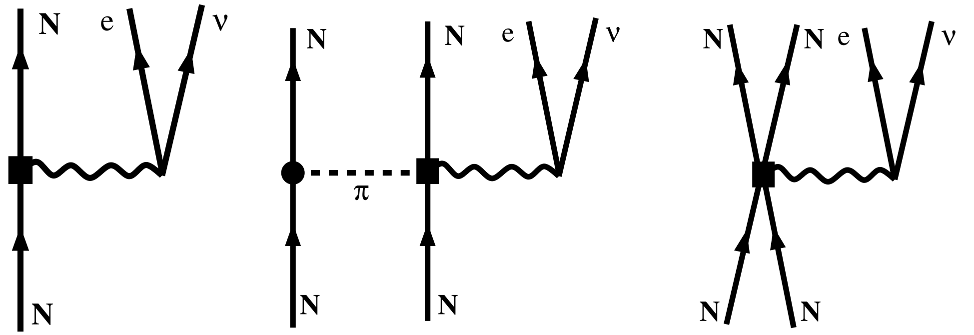
P. Gysbers[1,2], G. Hagen[3,4*], J. D. Holt[1], G. R. Jansen[3,5], T. D. Morris[3,4,6], P. Navrátil[1], T. Papenbrock[3,4], S. Quaglioni[7], A. Schwenk[8,9,10], S. R. Stroberg[1,11,12] and K. A. Wendt[7]

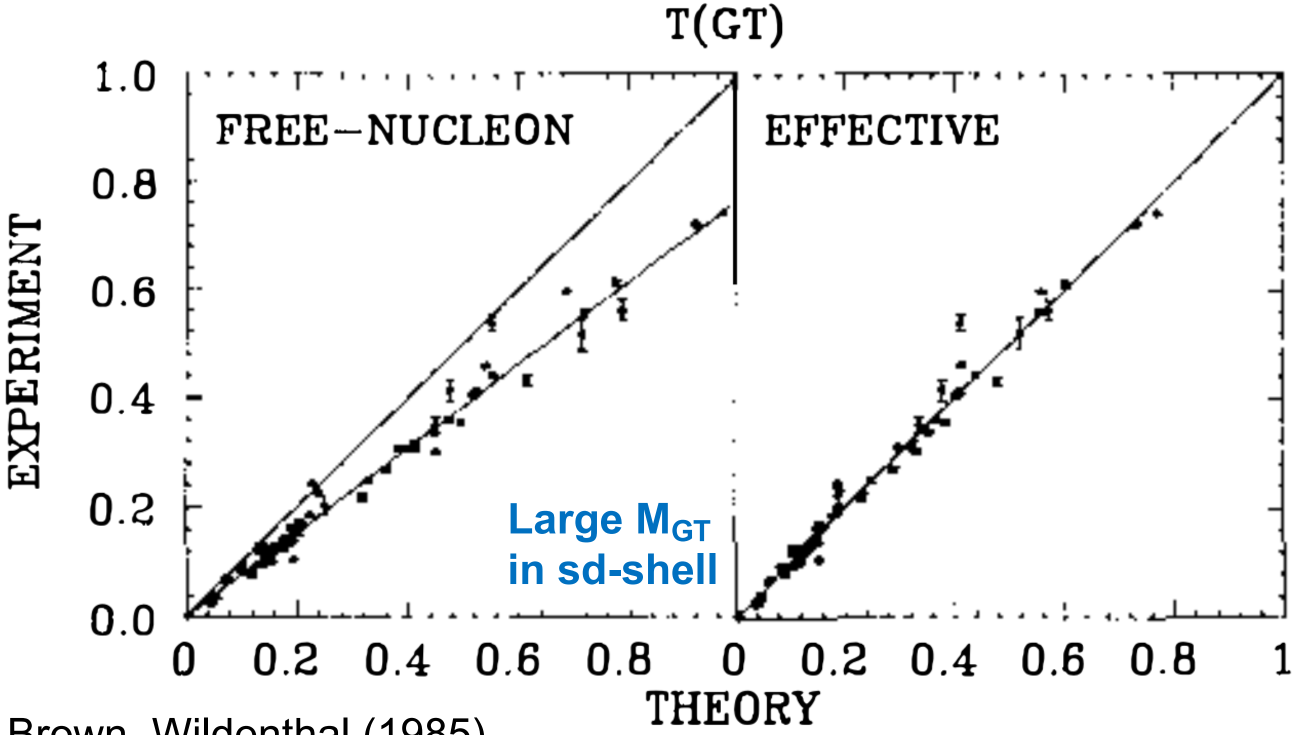
Beta-Decay "Puzzle": Quenching of g_A

Long-standing problem in weak decays: experimental values systematically smaller than theory

$$M_{\mathrm{GT}} = g_A \langle f | \mathcal{O}_{\mathrm{GT}} | i \rangle \quad \mathcal{O}_{\mathrm{GT}} = \mathcal{O}^{1\mathrm{b}}_{\sigma\tau} + \mathcal{O}^{2\mathrm{b}}_{2BC}$$

Using $g_A^{\mathrm{eff}} \approx 0.77 \times g_A^{\mathrm{free}}$ agrees with data





Brown, Wildenthal (1985)

- Missing wavefunction correlations
- Renormalized VS operator?
- Neglected two-body currents?
- Model-space truncations?

Explore in ab initio framework

Large-Scale Efforts for Ab Initio GT Transitions

Calculate **large GT matrix elements**

$$M_{\mathrm{GT}} = g_A \langle f | \mathcal{O}_{\mathrm{GT}} | i \rangle$$

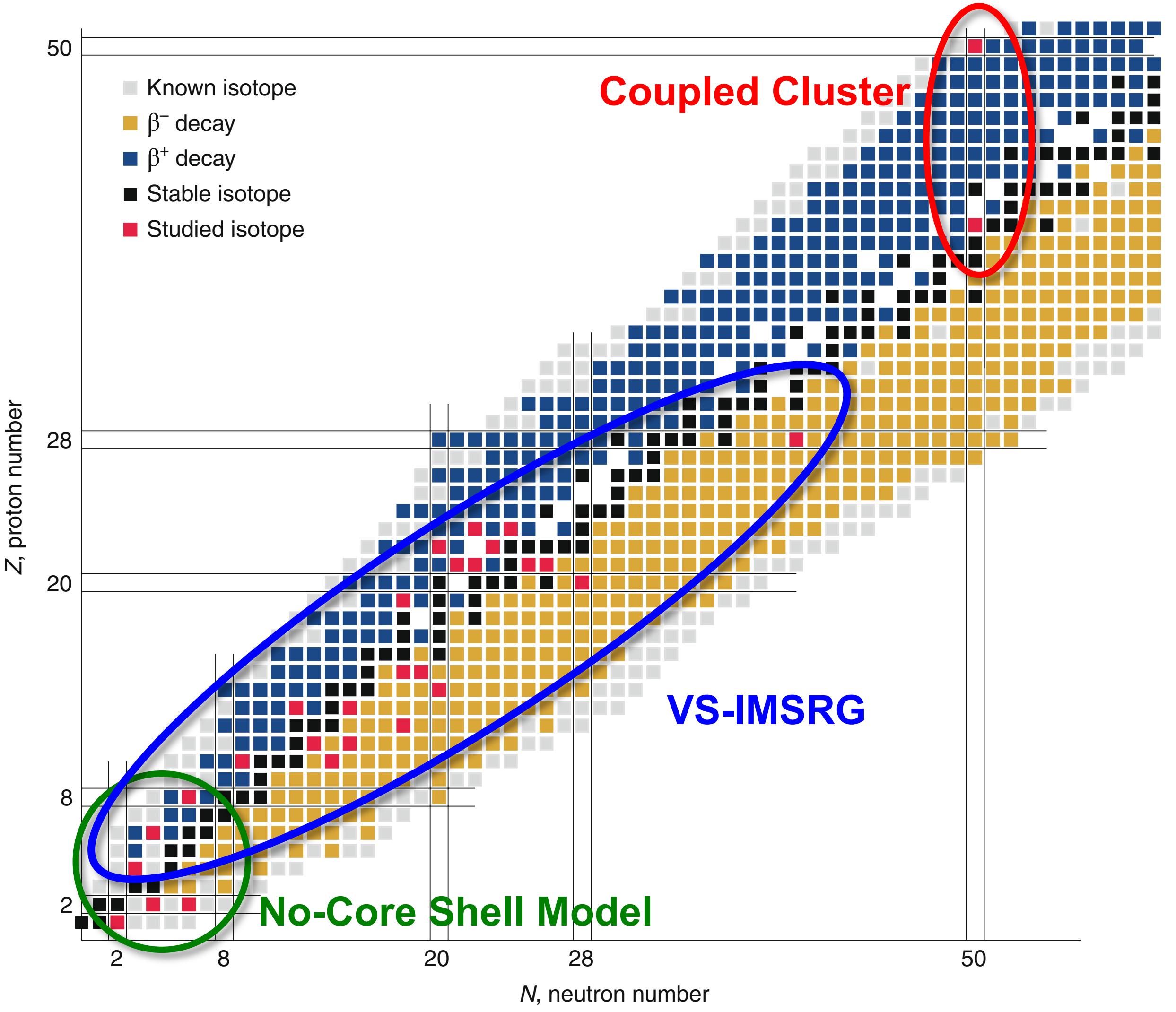
$$\mathcal{O}_{\mathrm{GT}} = \mathcal{O}_{\sigma\tau}^{1\mathrm{b}} + \mathcal{O}_{2BC}^{2\mathrm{b}}$$

- Light, medium, and heavy regions
- Benchmark different ab initio methods
- Range of NN+3N forces
- Consistent inclusion of 2BC

NUCLEAR PHYSICS

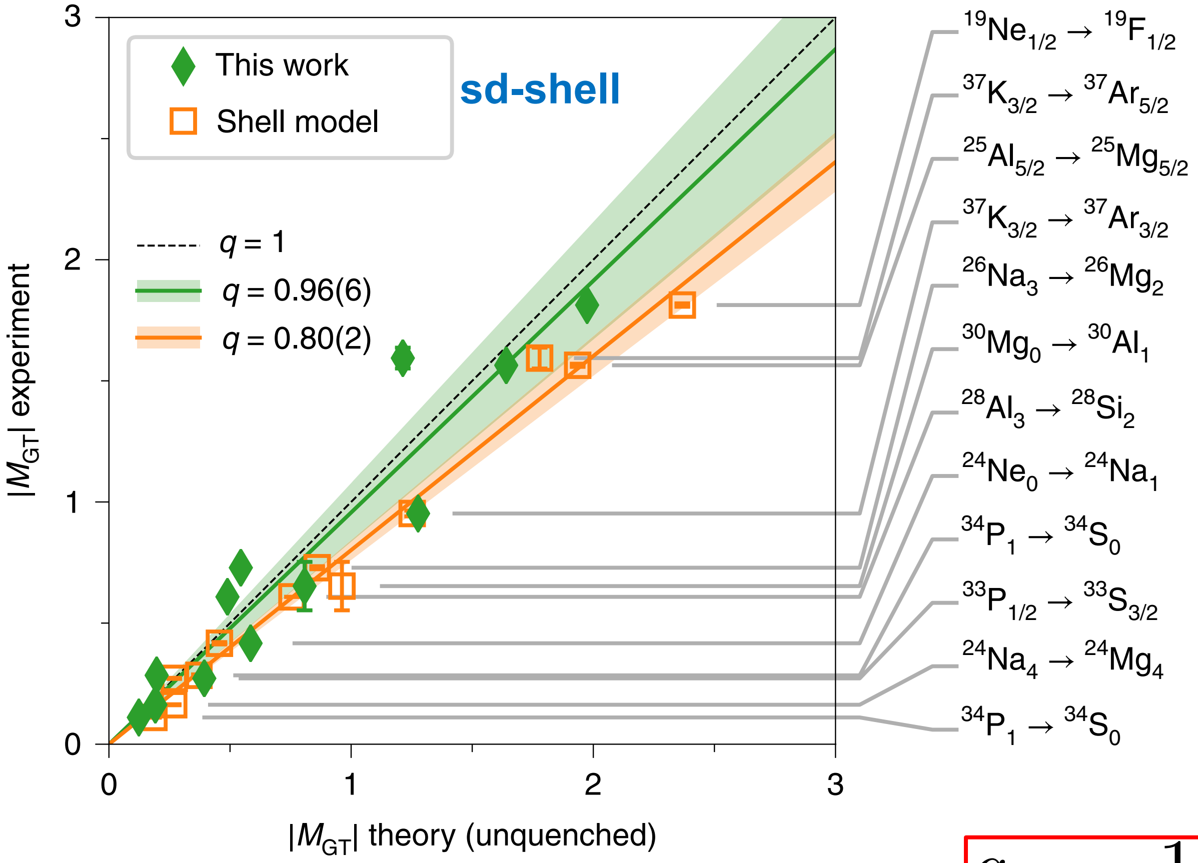
Beta decay gets the ab initio treatment

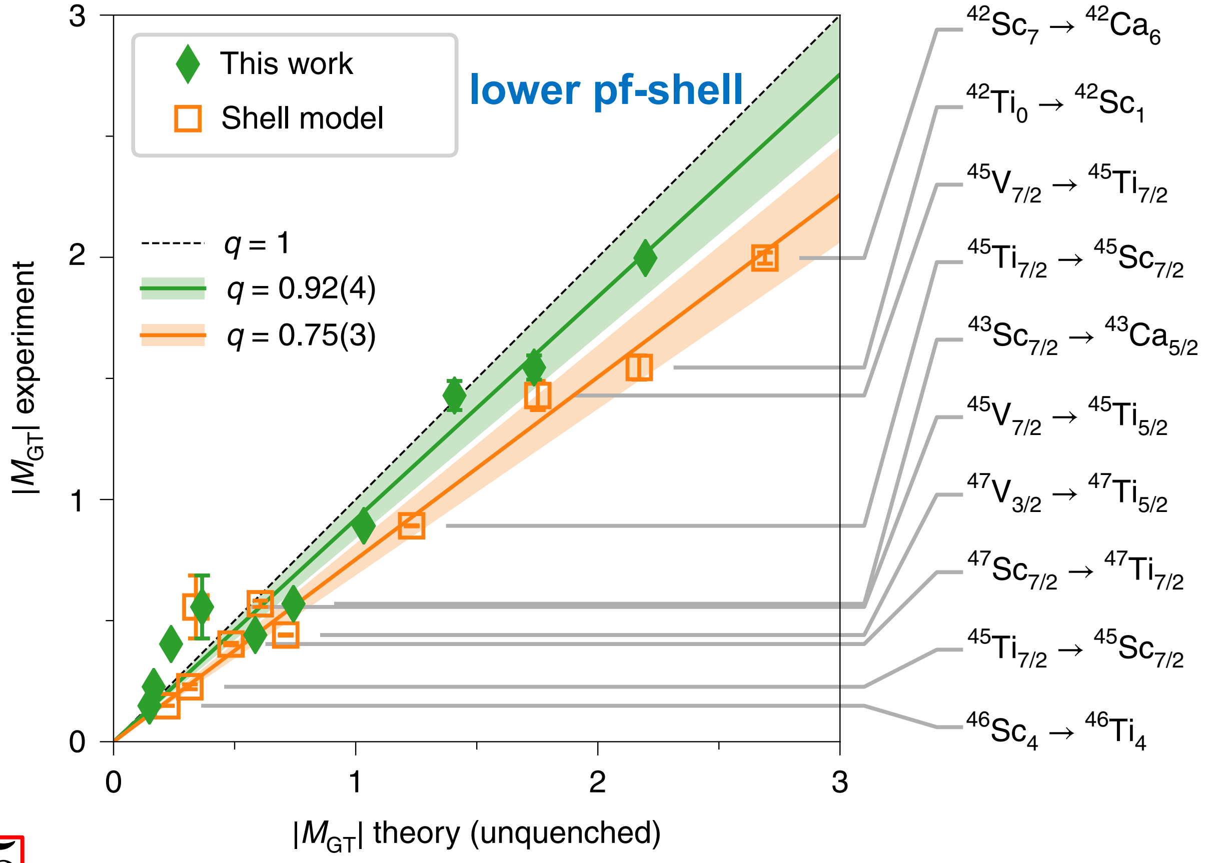
One of the fundamental radioactive decay modes of nuclei is β decay. Now, nuclear theorists have used first-principles simulations to explain nuclear β decay properties across a range of light- to medium-mass isotopes, up to ^{100}Sn.



Solution to g_A-Quenching Problem

VS-IMSRG calculations throughout sd and pf shells





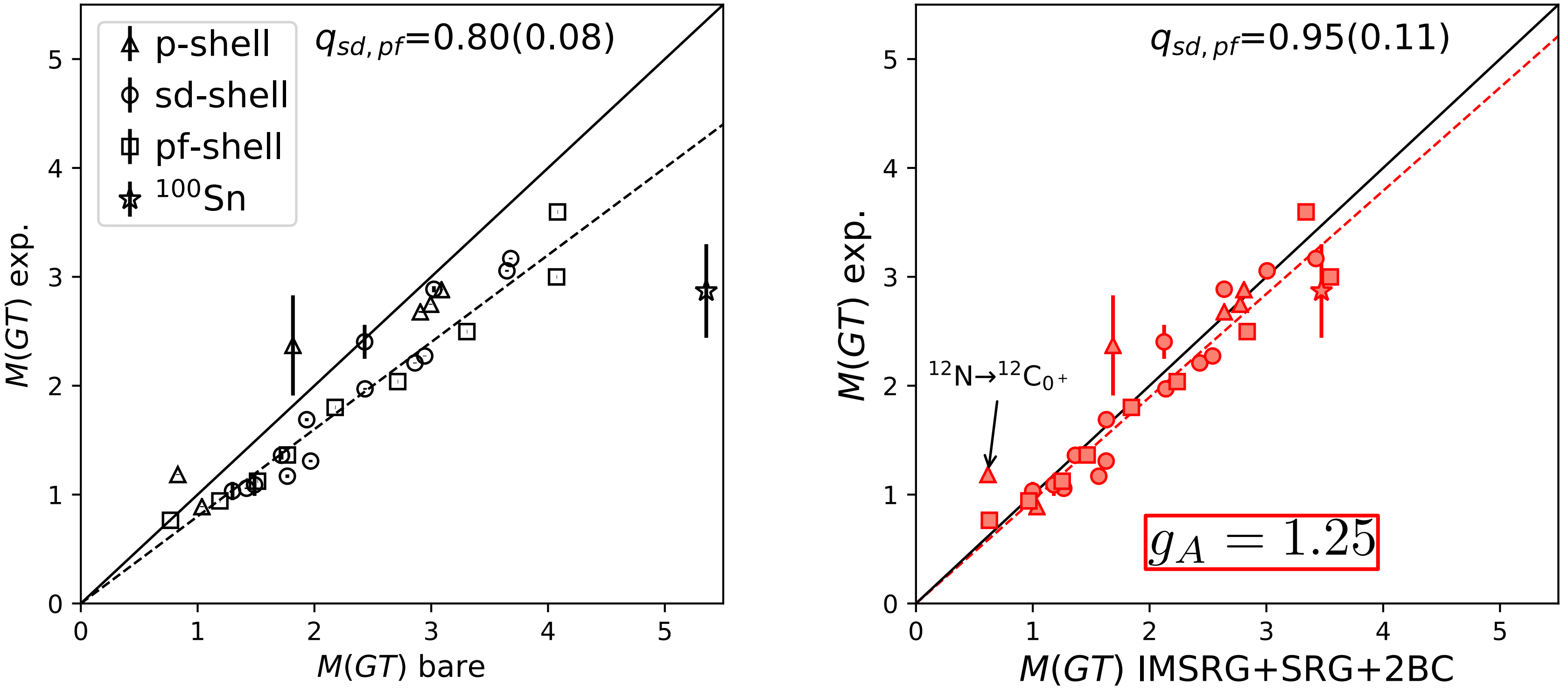
$$\boxed{g_A = 1.25}$$

Ab initio calculations across the chart explain data with unquenched g_A

Refine results: improvements in forces and many-body methods

Complete GT Picture: Light to ^{100}Sn

Ab initio calculations throughout sd and pf shells



Stroberg (2021)

Ab initio calculations across the chart explain data with unquenched g_A

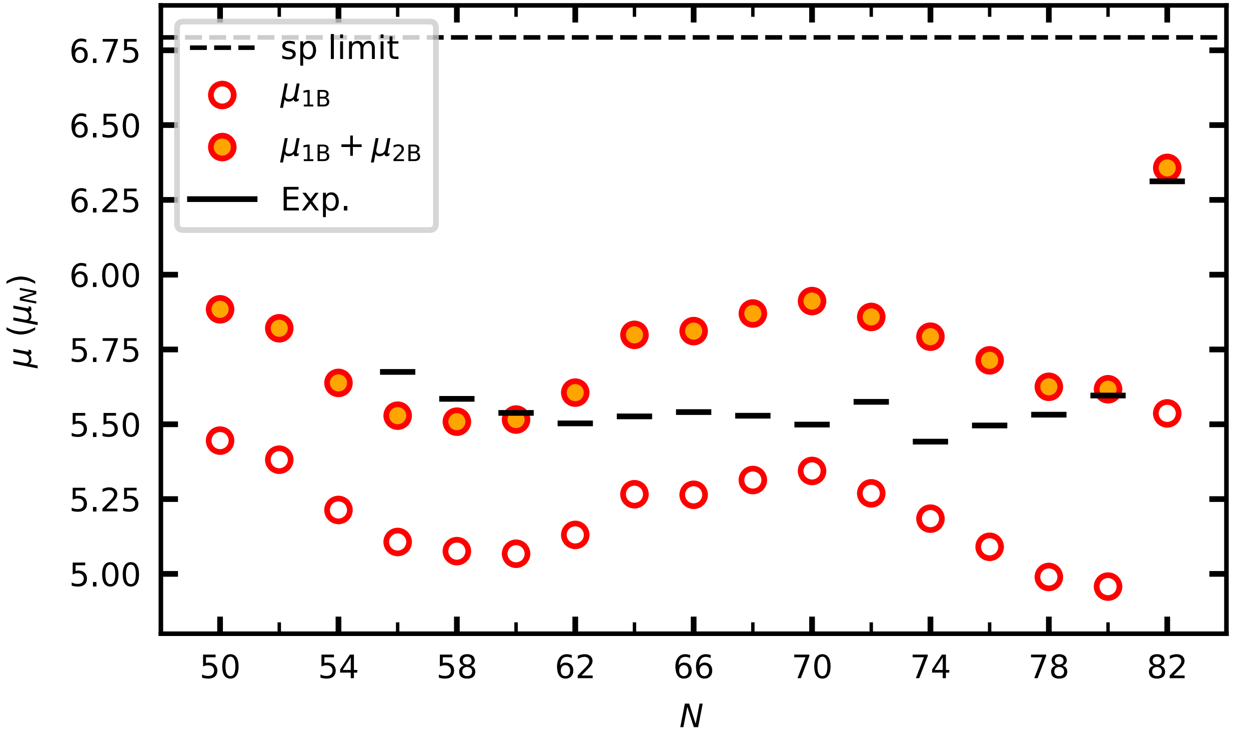
Including p-shell: q=0.99(21)

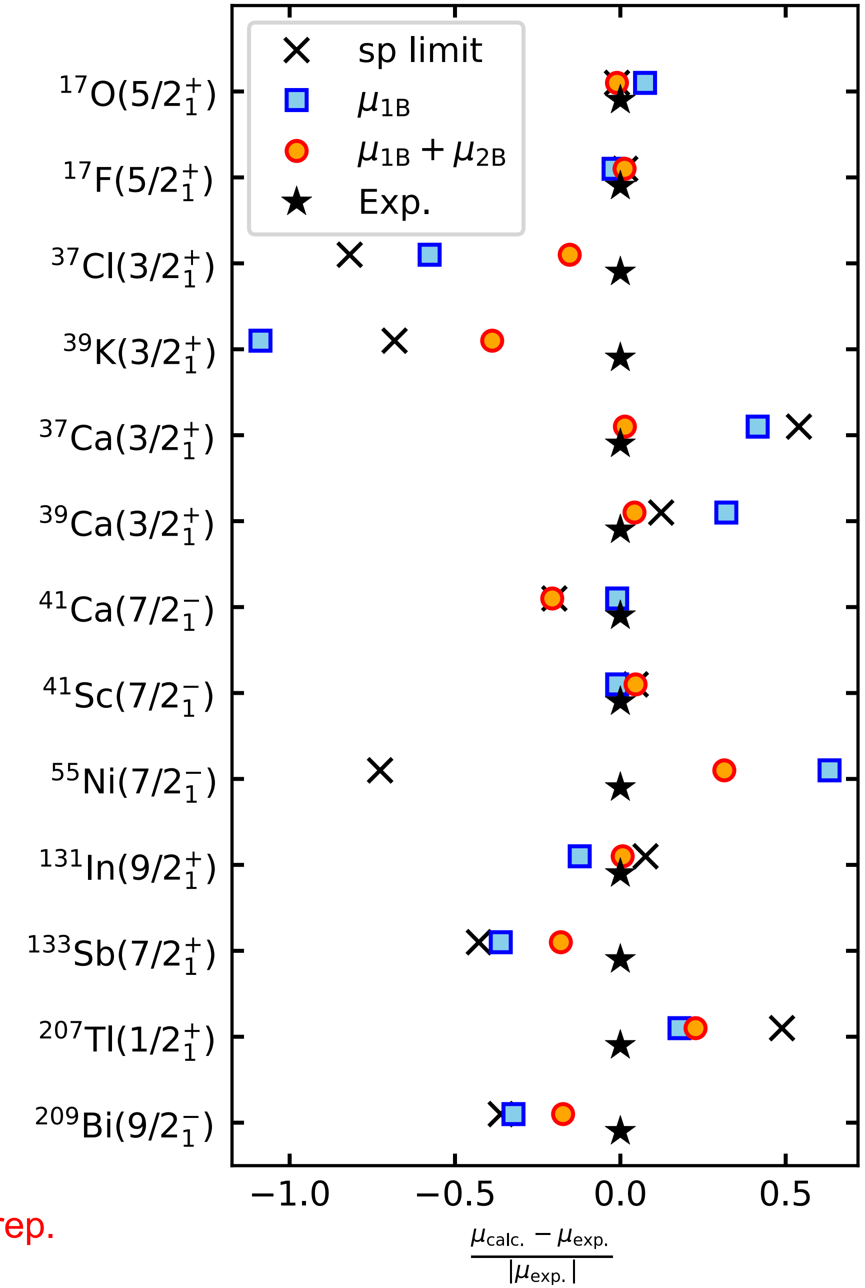
Impact of Two-Body M1 Currents

Ab initio calculations throughout the nuclear chart

Including 2bc consistent with input forces

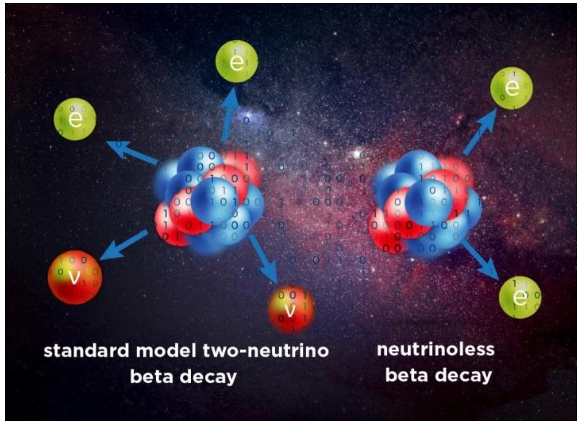
Magnetic moments significantly improved



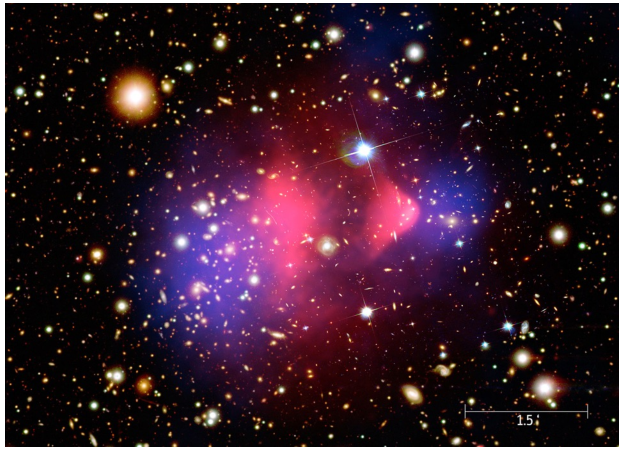


T. Miyagi et al, in prep.

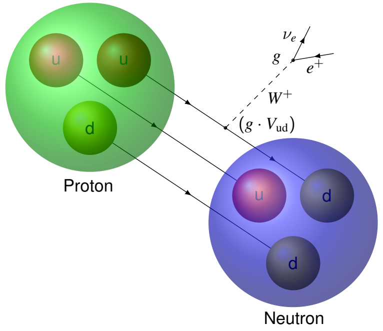
Applications to Searches for BSM Physics



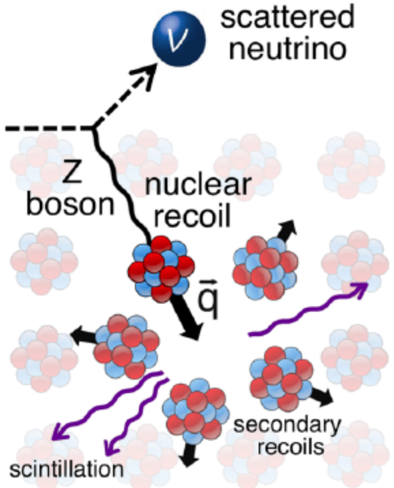
Neutrinoless double beta decay



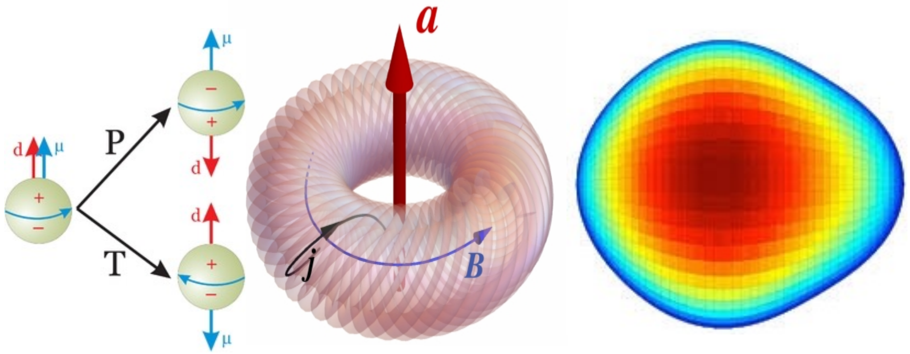
Dark matter direct detection



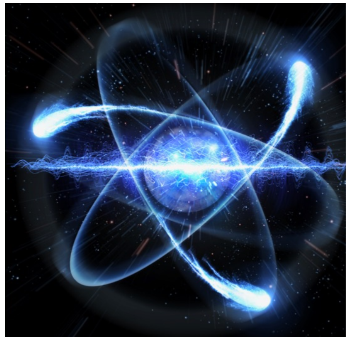
Superallowed Fermi transitions



Neutrino scattering



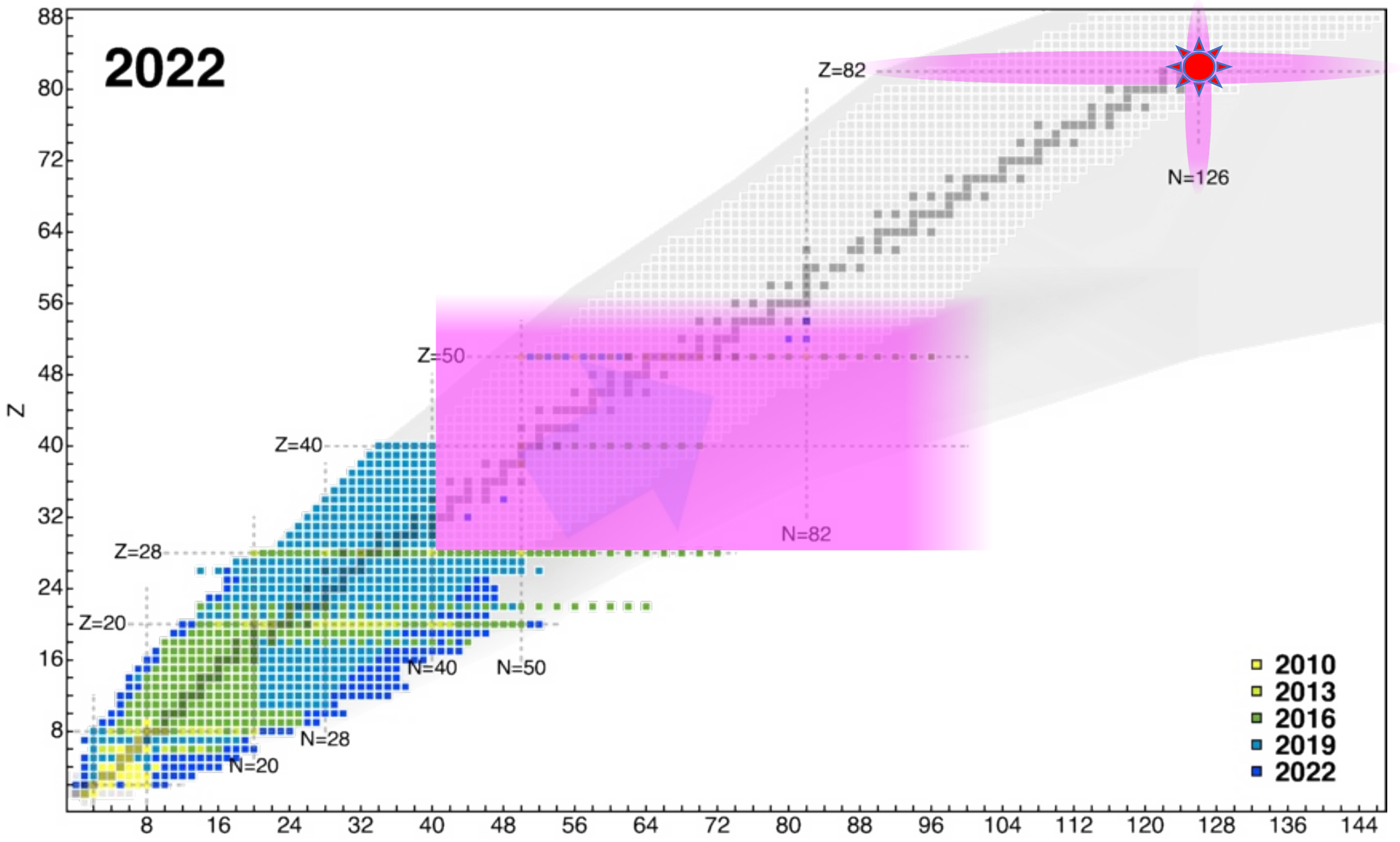
Symmetry-violating moments



Atomic theory

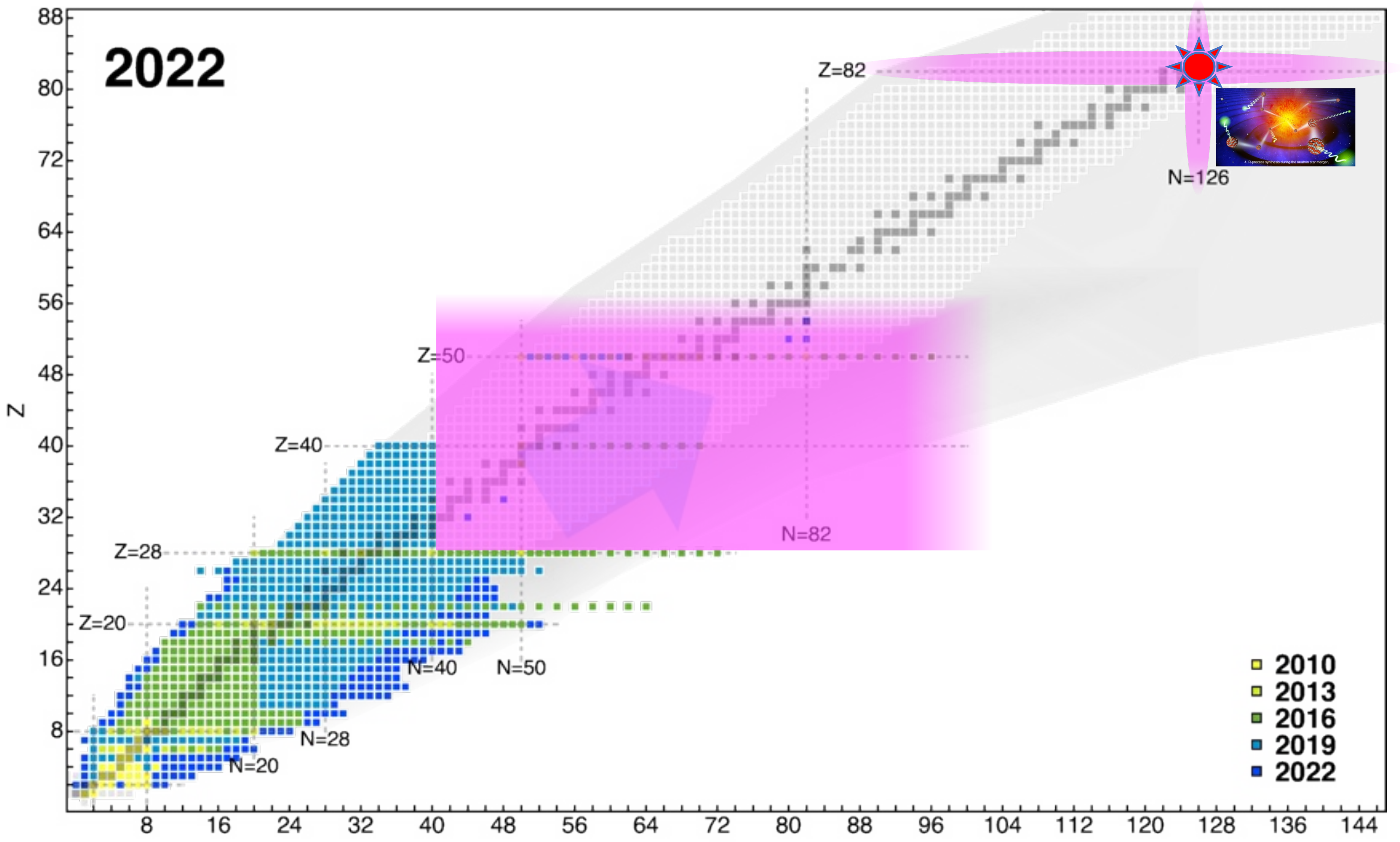
Where to Next? Five Predictions for ARIS 2026

What will be the major ab initio accomplishments in the next 3 years?



Where to Next? Five Predictions for ARIS 2026

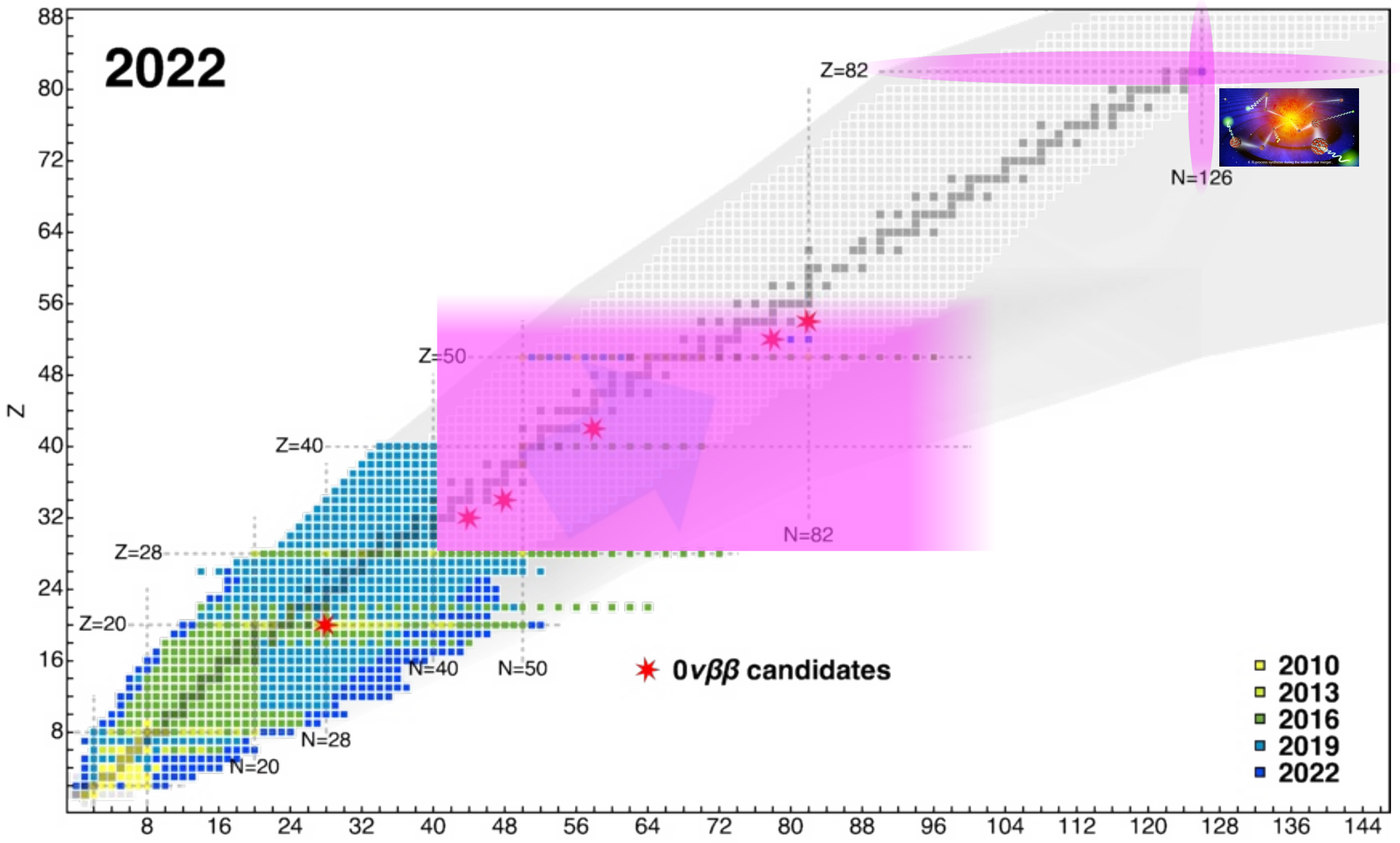
What will be the major ab initio accomplishments in the next 3 years?



1) Inputs for r-process

Where to Next? Five Predictions for ARIS 2026

What will be the major ab initio accomplishments in the next 3 years?



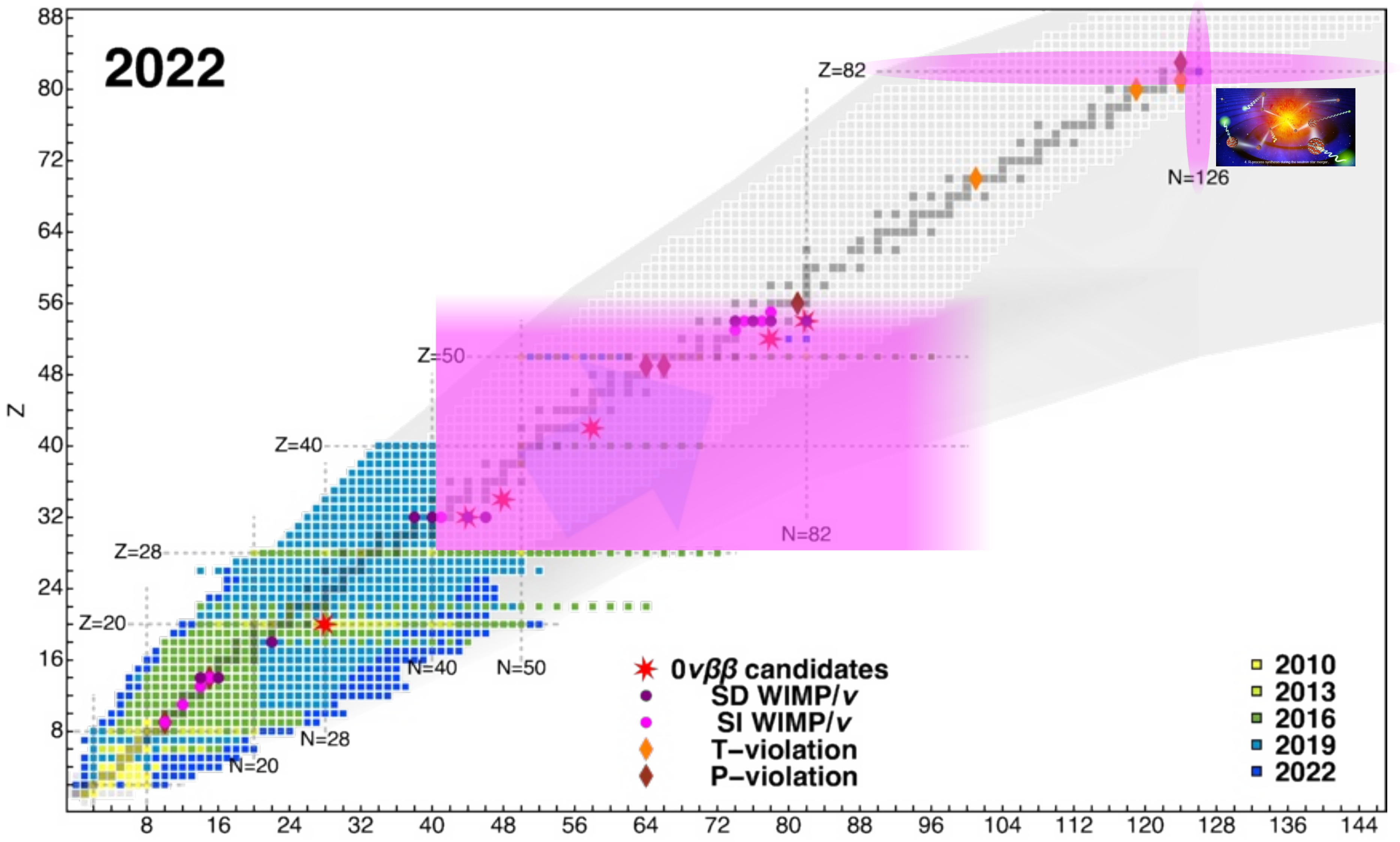
1) Inputs for r-process

2) $0\nu\beta\beta$ decay + th. errors

TRIUMF

Where to Next? Five Predictions for ARIS 2026

What will be the major ab initio accomplishments in the next 3 years?



1) Inputs for r-process

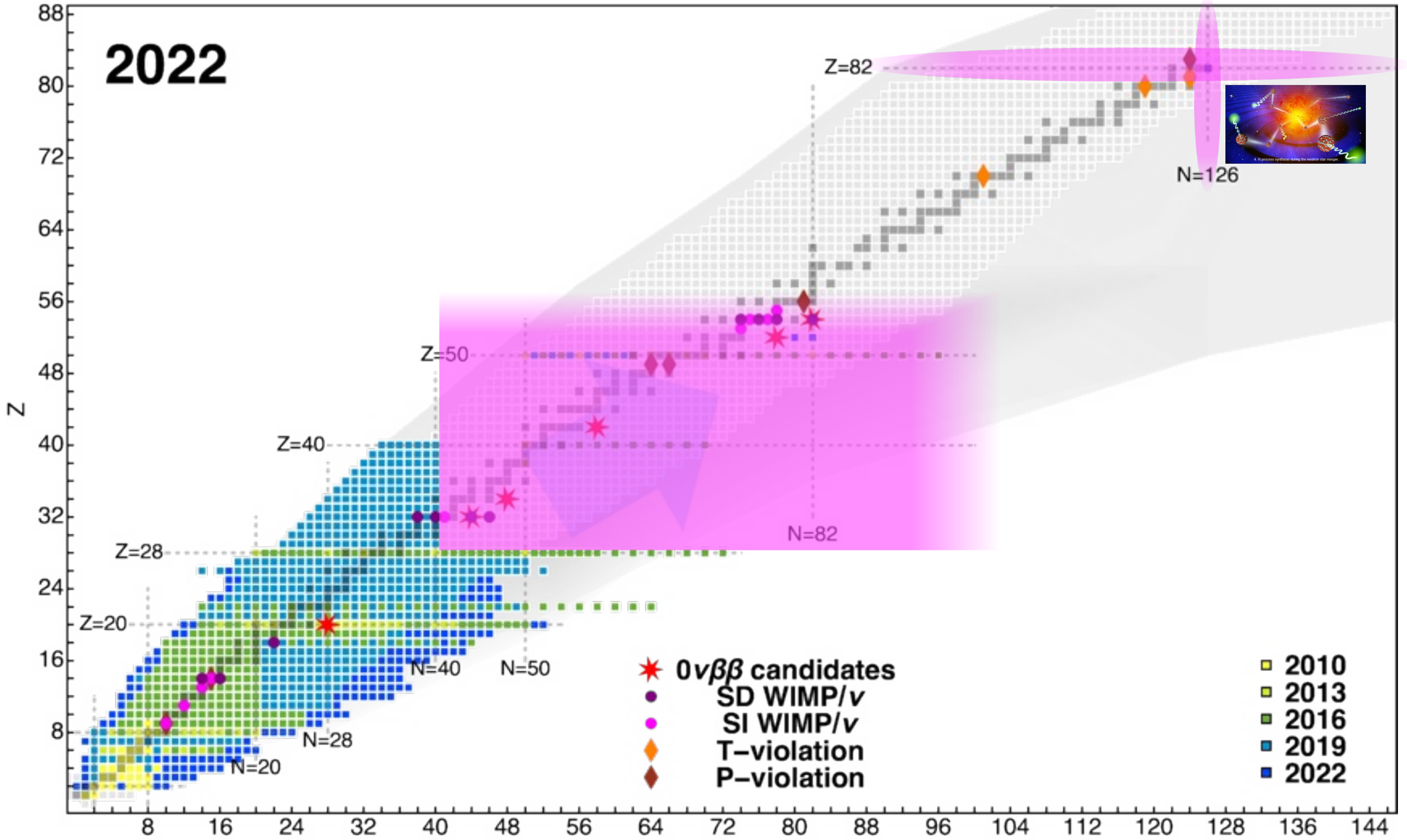
2) $0\nu\beta\beta$ decay + th. errors

3) Symmetry violation

See talk:
R. F. Garcia-Ruiz

Where to Next? Five Predictions for ARIS 2026

What will be the major ab initio accomplishments in the next 3 years?



1) Inputs for r-process

2) $0\nu\beta\beta$ decay + th. errors

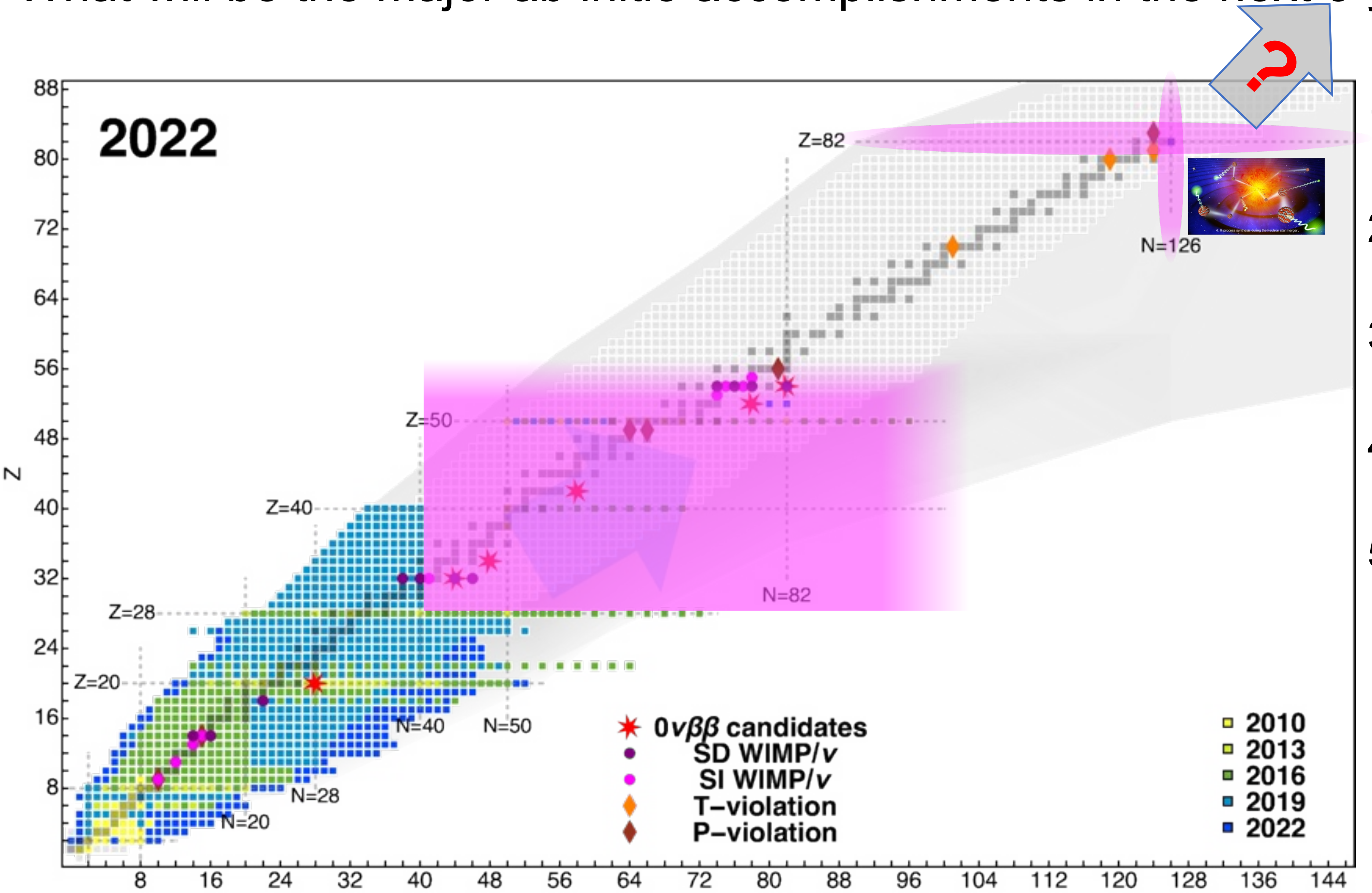
3) Symmetry violation

4) Global optical potential

TRIUMF

Where to Next? Five Predictions for ARIS 2026

What will be the major ab initio accomplishments in the next 3 years?



1) Inputs for r-process

2) $0\nu\beta\beta$ decay + th. errors

3) Symmetry violation

4) Global optical potential

5) Superheavy region (?)

Let's see in 2026!

TRIUMF

Present and Future for Ab Initio Theory

Nuclear Structure/Astrophysics

Development of forces and currents

Ab initio to ^{208}Pb: neutron skin, r-process

Dripline predictions to medium-masses

Evolution of magic numbers:

  masses, radii, spectra, EM transitions

Multi-shell theory:

  Islands of inversion, forbidden decays

Nuclear EOS/Neutron star properties

Atomic systems

Fundamental Symmetries/BSM Physics

EW operators: GT quenching, muon capture

$0\nu\beta\beta$ decay matrix elements + DGT/ECEC/Dg

WIMP-Nucleus scattering for dark matter detection

Coherent elastic neutrino-nucleus scattering

Superallowed Fermi transitions

Symmetry-violating moments: EDM, anapole, Schiff

Work in progress

Higher-order many-body physics: IMSRG(3)

Monte Carlo shell model diagonalization

Extension to superheavy nuclei

TRIUMF

THE UNIVERSITY OF BRITISH COLUMBIA

McGill UNIVERSITY

T. Miyagi, B. S. Hu, L. Jokiniemi

A. Belley, I. Ginnett, C. G. Payne

M. Bruneault, J. Padua

S. Leutheusser

E. Love

K. Evidence, D. Kush

G. Tenkila, H. Patel, V. Chand

B. Wong, X. Cao

S. R. Stroberg N. Vassh

TECHNISCHE UNIVERSITÄT DARMSTADT — A. Schwenk

THE UNIVERSITY of TENNESSEE KNOXVILLE — G. Hagen, T. Papenbrock

MICHIGAN STATE UNIVERSITY — J.M. Yao, H. Hergert

COLORADO SCHOOL OF MINES — M. Martin, K. G. Leach

Massachusetts Institute of Technology — R. F. Garcia-Ruiz

UNIVERSITAT DE BARCELONA — J. Menéndez

THE UNIVERSITY of NORTH CAROLINA at CHAPEL HILL — J. Engel

TEXAS A&M UNIVERSITY — J. W. Holt

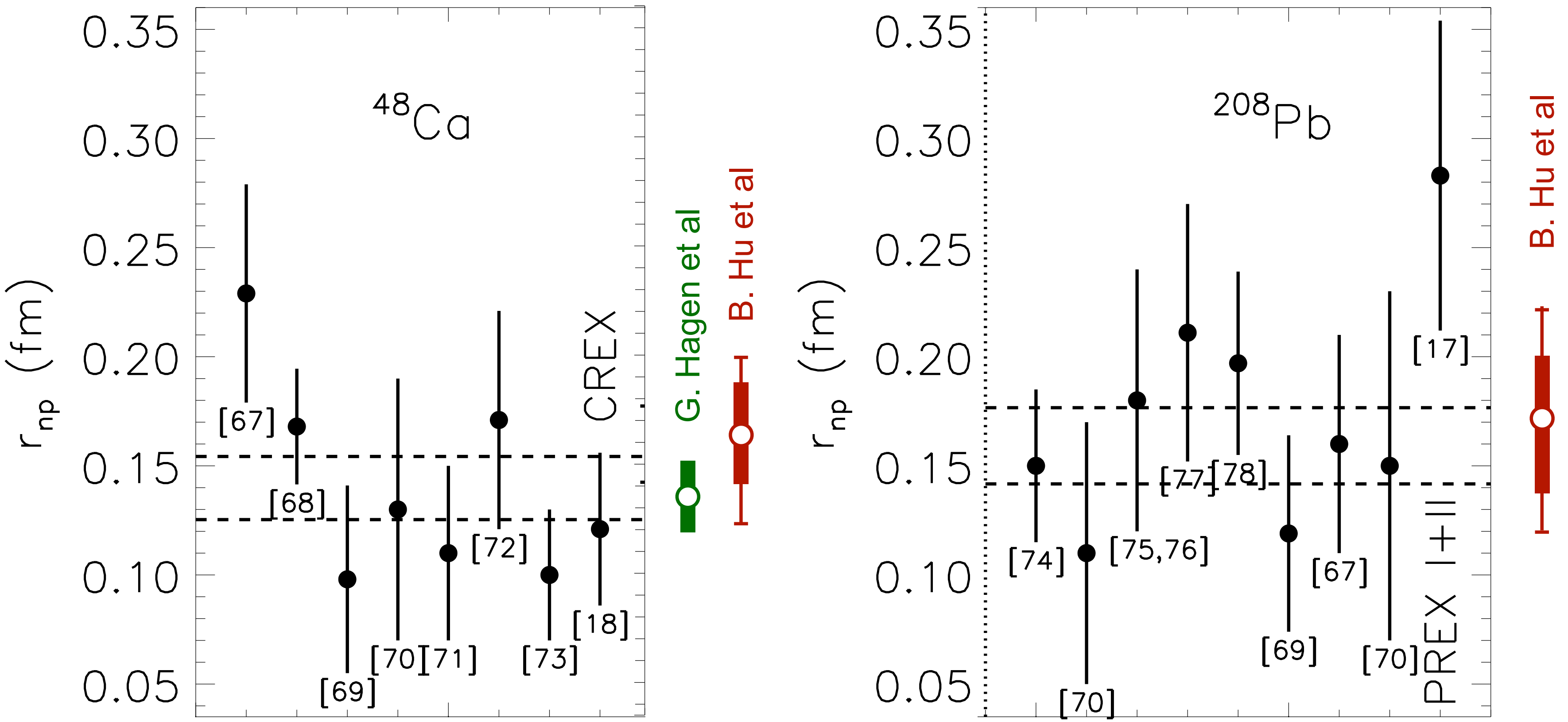
TRIUMF

Confrontation with R_{skin} of ^{48}Ca

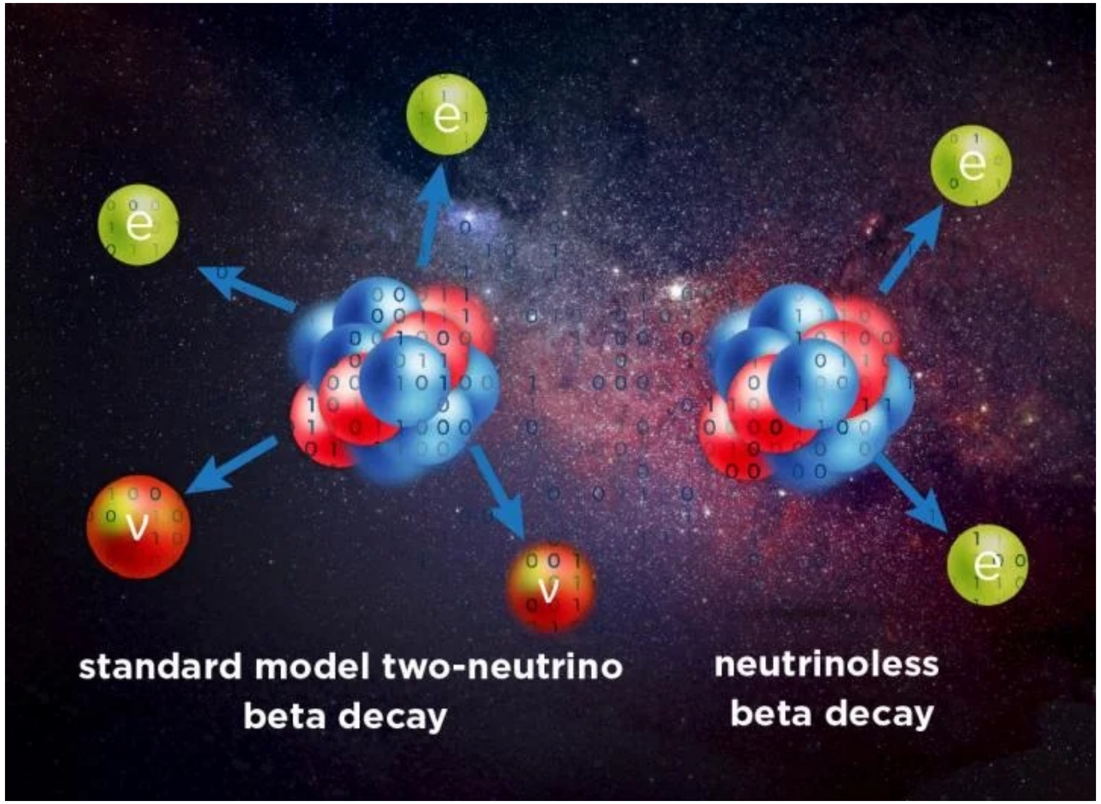
Newly extracted neutron skin in ^{48}Ca

Use same 34 interactions – predictions in good agreement with CREX result

Constraints on Nuclear Symmetry Energy Parameters
J. Lattimer (2023)



Neutrinoless Double Beta Decay NMEs for Major Players: ^{76}Ge, (^{100}Mo), ^{130}Te, ^{136}Xe



Ab Initio Treatment of Collective Correlations and the Neutrinoless Double Beta Decay of ^{48}Ca

J. M. Yao, B. Bally, J. Engel, R. Wirth, T. R. Rodríguez, and H. Hergert
Phys. Rev. Lett. **124**, 232501 – Published 11 June 2020

Ab Initio Neutrinoless Double-Beta Decay Matrix Elements for ^{48}Ca, ^{76}Ge, and ^{82}Se

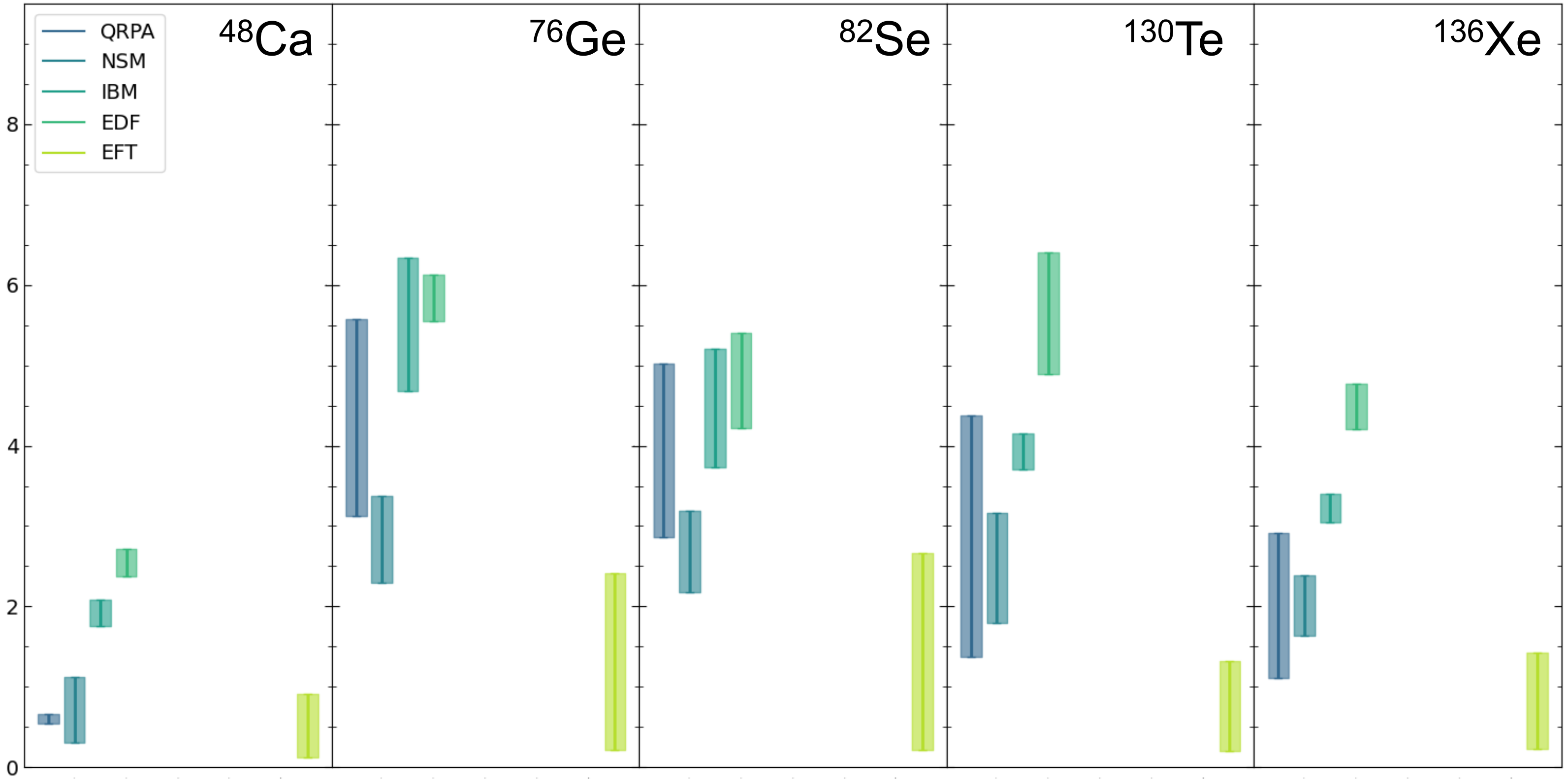
A. Belley, C. G. Payne, S. R. Stroberg, T. Miyagi, and J. D. Holt
Phys. Rev. Lett. **126**, 042502 – Published 29 January 2021

Coupled-Cluster Calculations of Neutrinoless Double-β Decay in ^{48}Ca

S. Novario, P. Gysbers, J. Engel, G. Hagen, G. R. Jansen, T. D. Morris, P. Navrátil, T. Papenbrock, and S. Quaglioni
Phys. Rev. Lett. **126**, 182502 – Published 7 May 2021

Current Status of NMEs

Calculations to date from phenomenological models; large spread in results



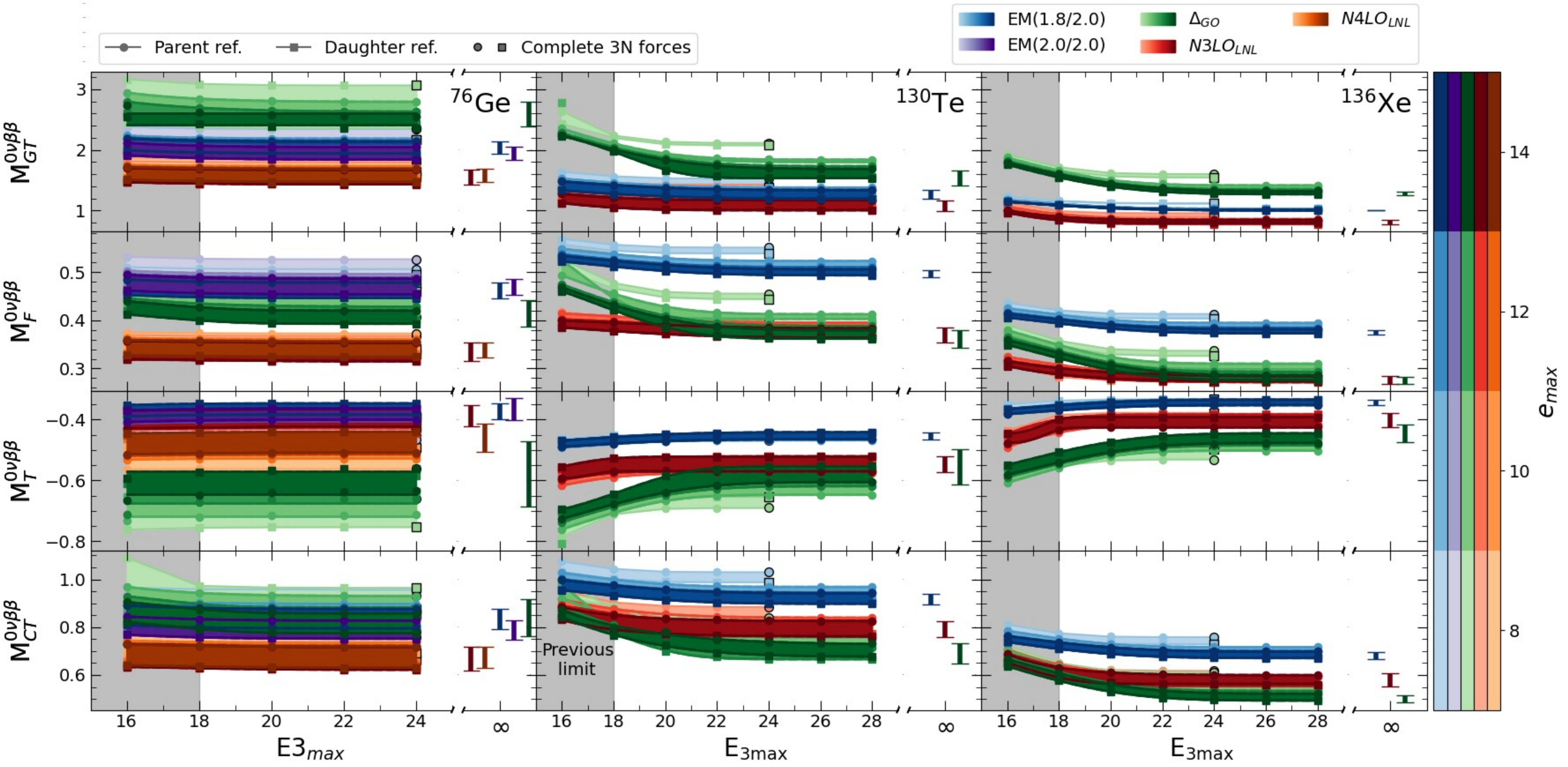
Compiled values from: Engel and Menéndez (2017); Brase et al, PRC (2022)

All models missing essential physics: correlations, single-particle levels, two-body currents

Address with ab initio theory

Ab Initio Predictions in Heavy Nuclei

Converged NMEs for major players in global searches: ^{76}Ge, ^{130}Te, ^{136}Xe



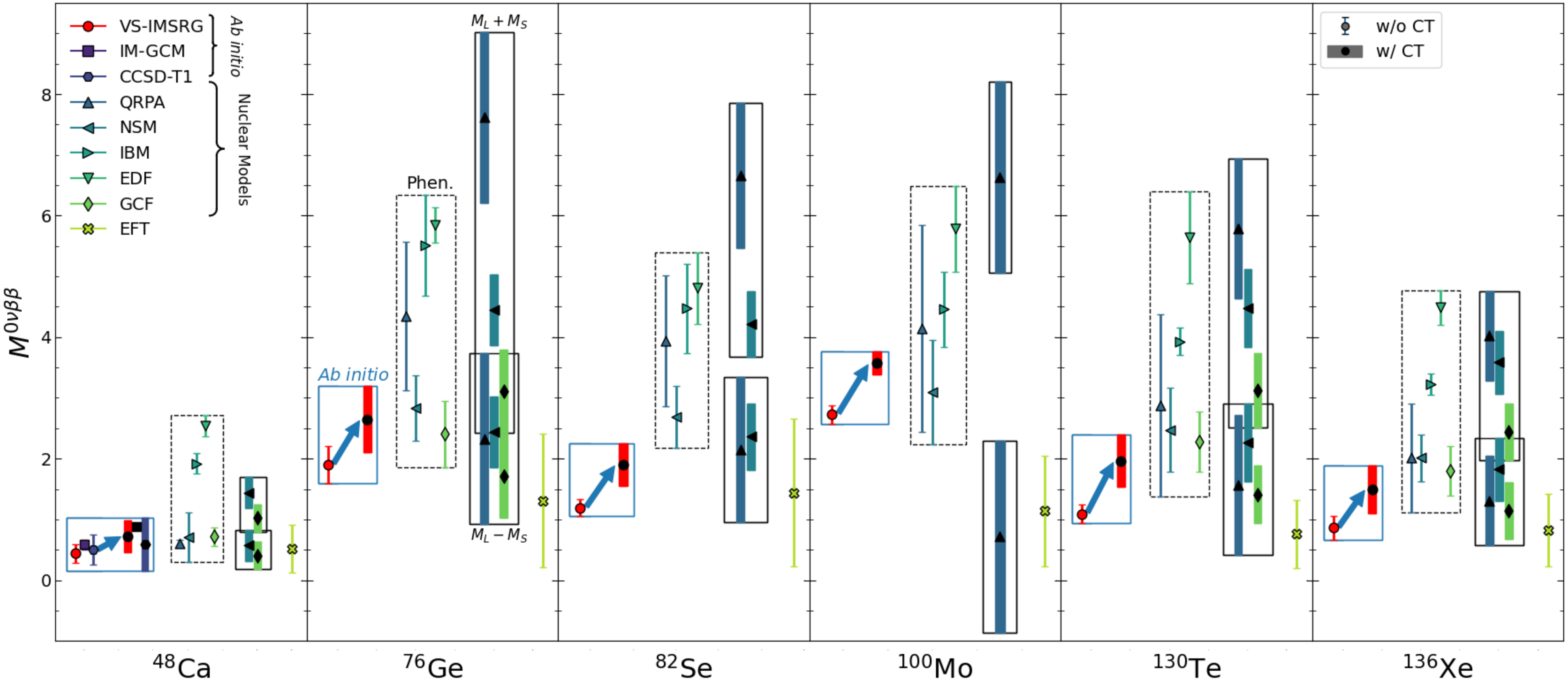
Belley et al, in prep

TRIUMF

Ab Initio Predictions in Heavy Nuclei

Converged NMEs for major players in global searches: ^{76}Ge, ^{100}Mo ^{130}Te, ^{136}Xe

Ab initio results: differences from models; **large NMEs strongly disfavored**

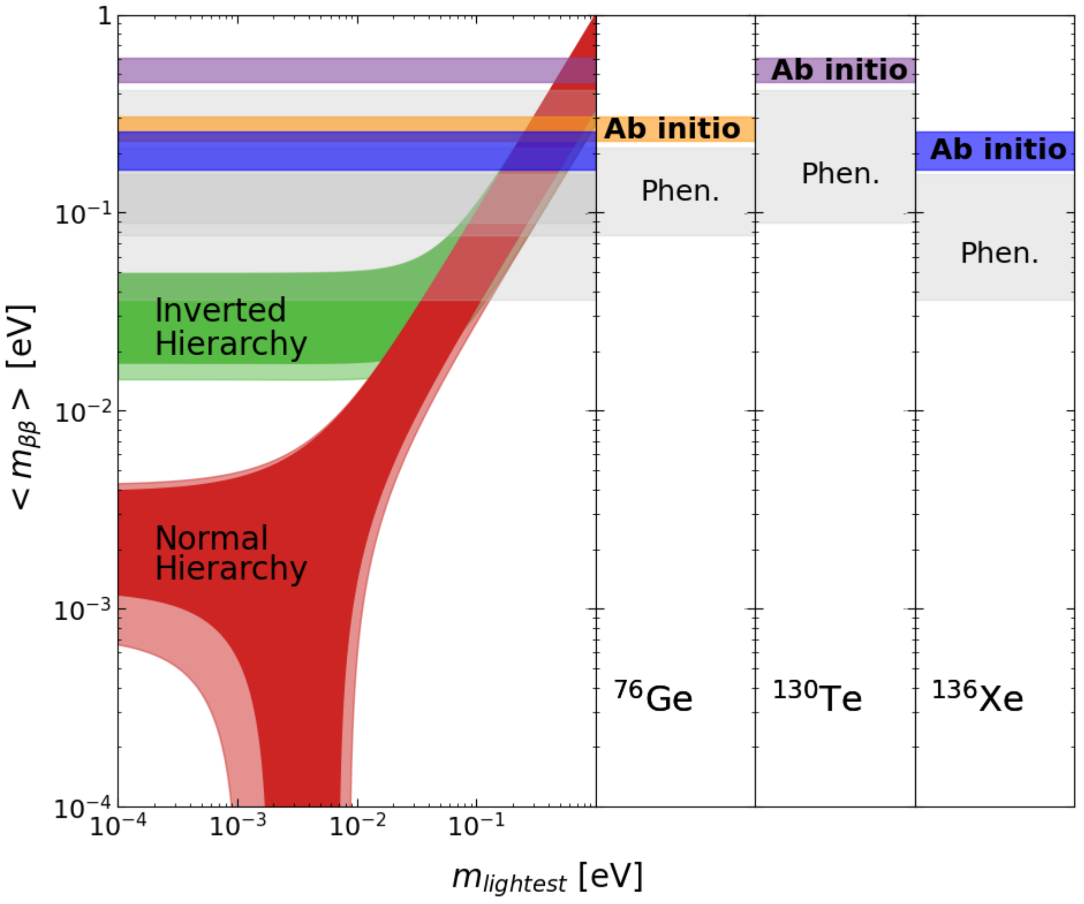


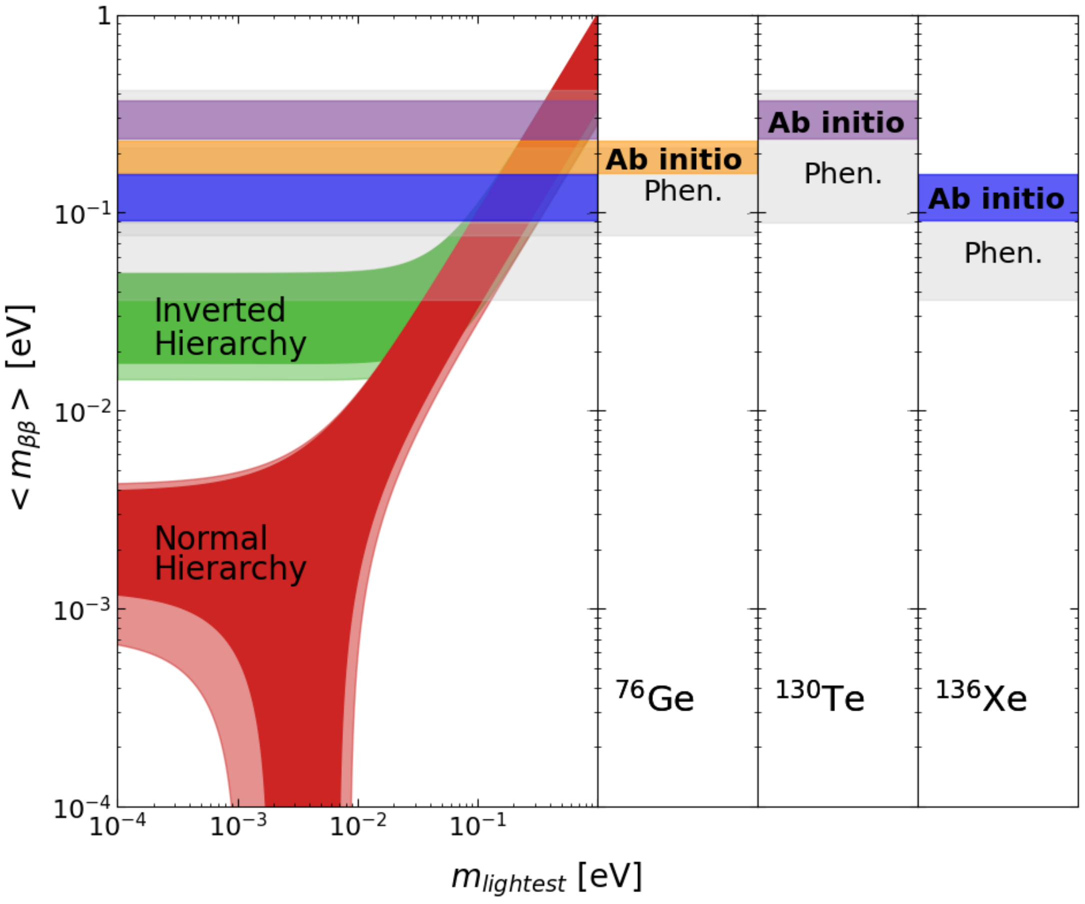
Belley et al, in prep

Impact of Ab Initio NMEs on Worldwide Searches

Impact for next-generation searches: Large matrix elements disfavored, lowers expected rates

Current experimental reach – improved with effects of contact term,





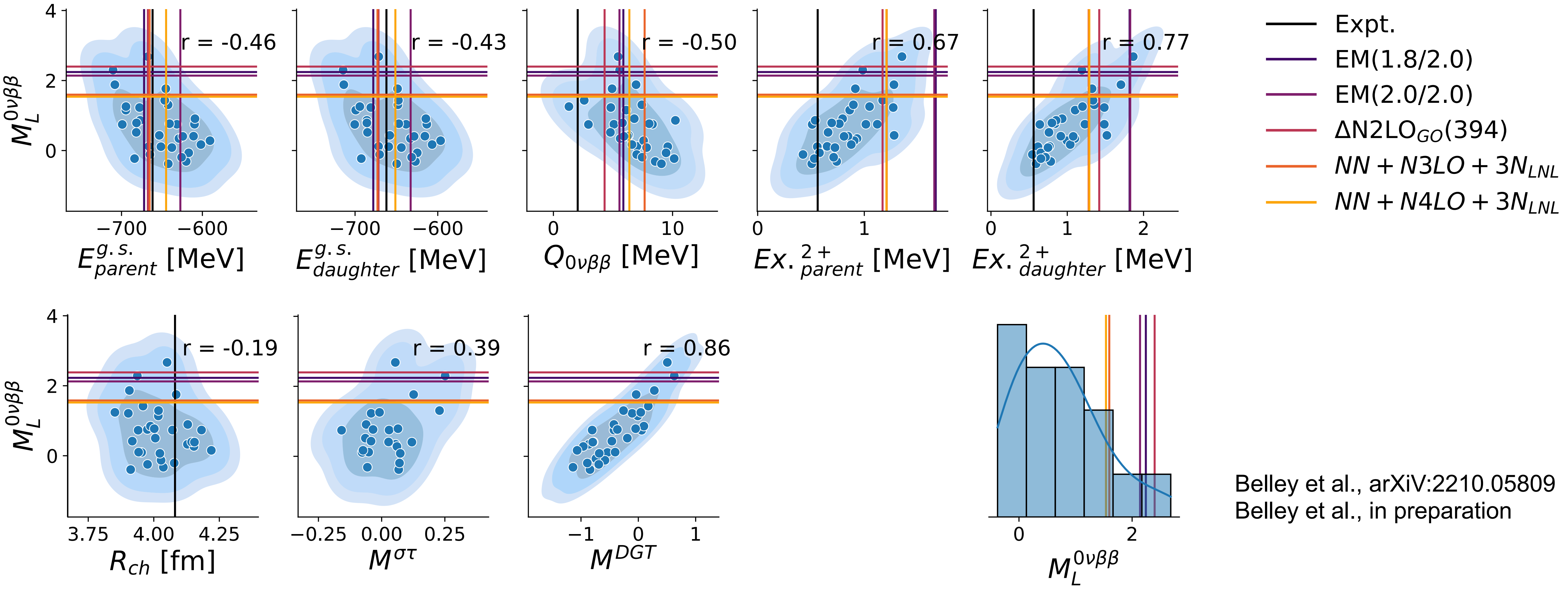
Not the end of the story: estimate three-body corrections + two-body currents

Belley et al, in prep

Strategy III: Correlation with Structure Observables

^{76}Ge: Explore correlations with other observables from systematic analysis (34 interactions)

Few clear correlations, except DGT



Belley et al., arXiV:2210.05809
Belley et al., in preparation

Maybe with first excited 2^+ states?

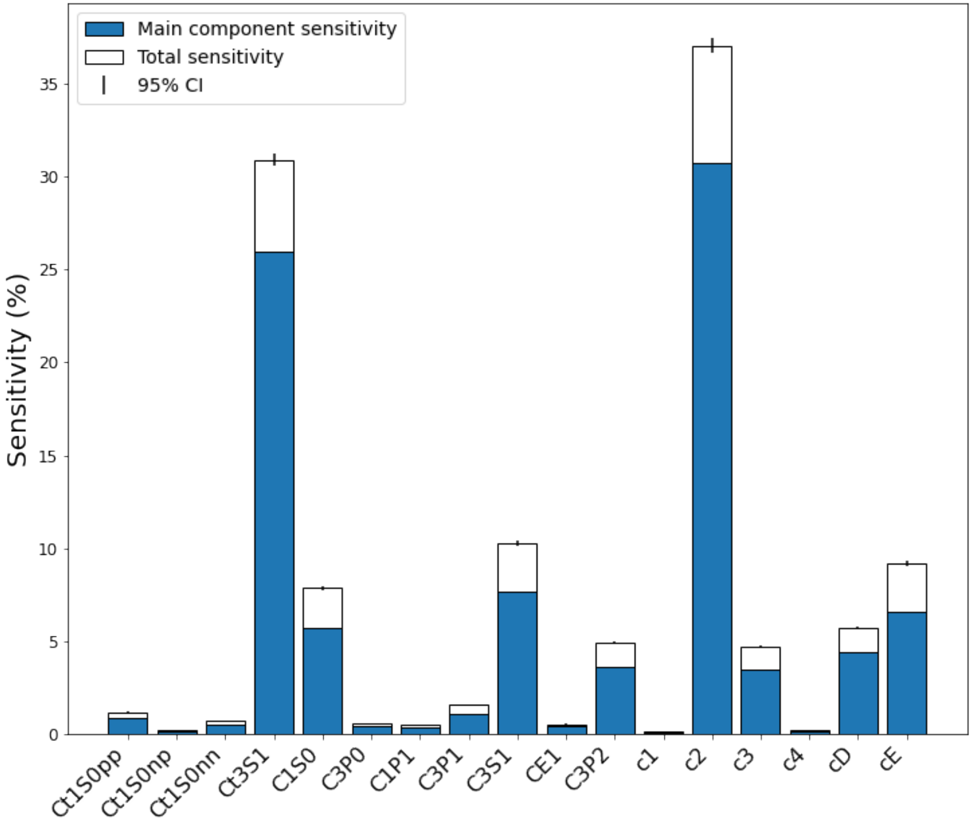
MM-DGP Emulator: Sensitivity Analysis

Explore correlations with other observables from systematic analysis (34 interactions)

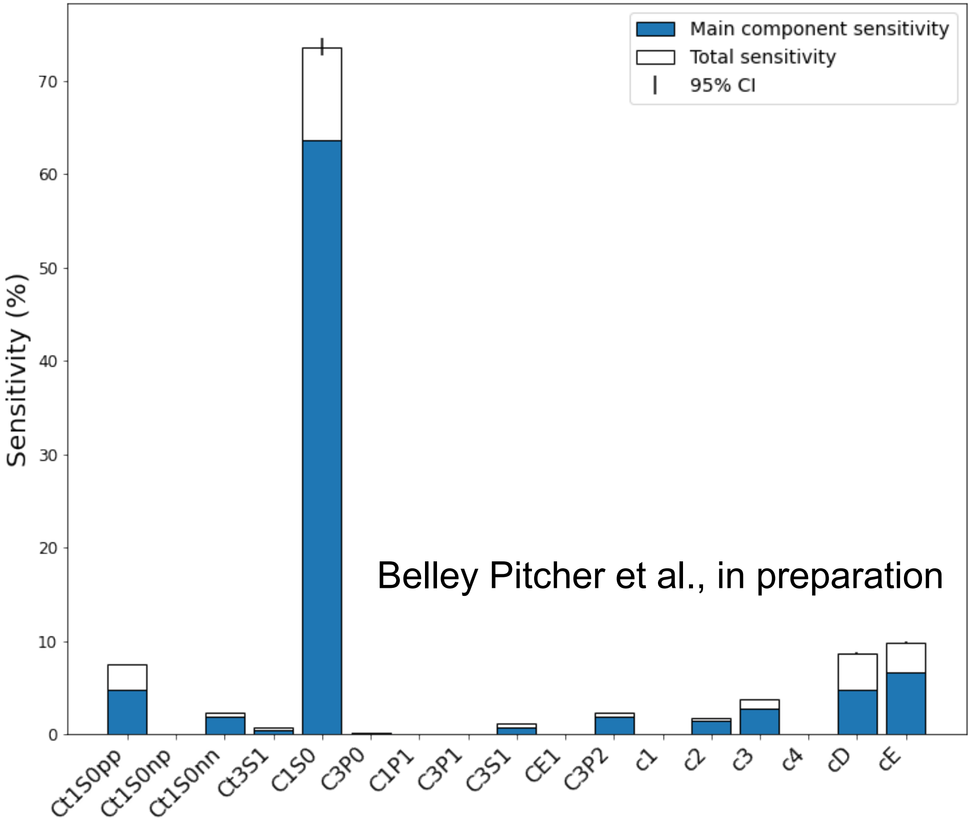
Similar sensitivity as found in ^{208}Pb study!

26

Ground state energies



$M_L^{0\nu}$

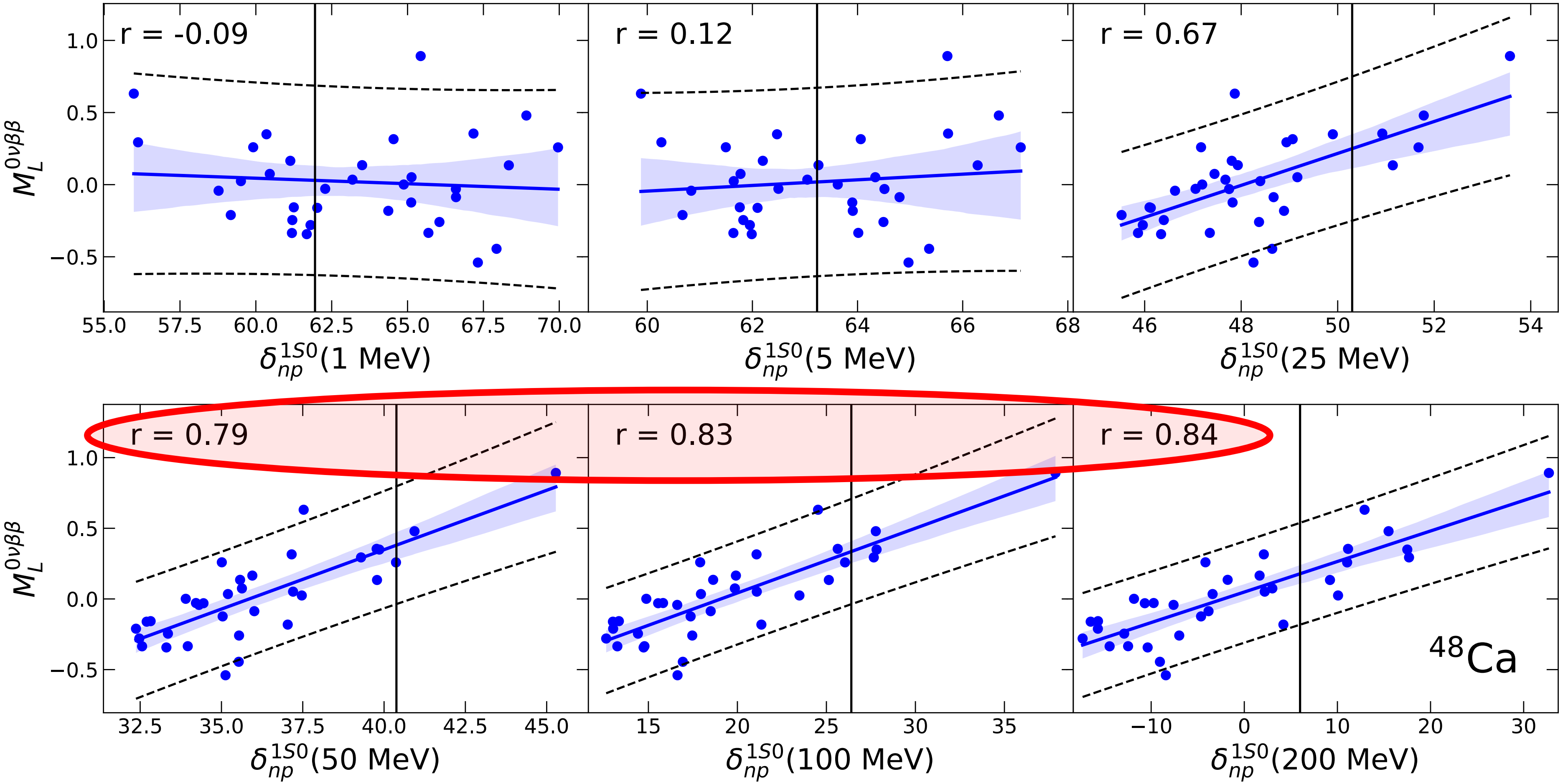


Highly sensitive to C1S0 – possible correlation with $^1S_0$ phase shift (observable!)

MM-DGP Emulator: Correlation w/ $^1S_0$ Phase Shift

Explore correlations with $^1S_0$ phse shift from 34 non-implausible interactions

Long-range component in ^{48}Ca

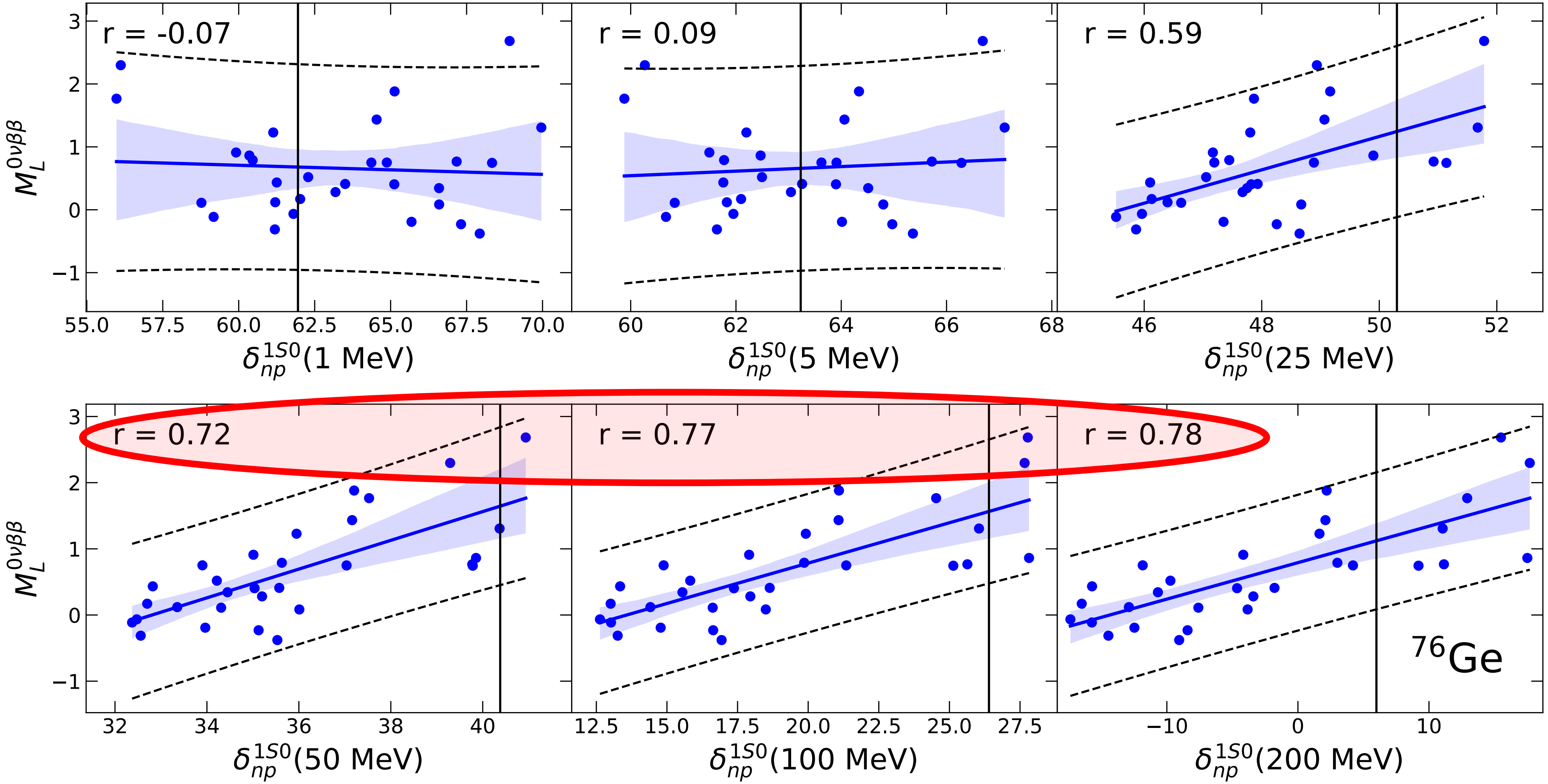


Clear correlation with (measured!) $^1S_0$ phase shift at high scattering energies

MM-DGP Emulator: Correlation w/ $^1S_0$ Phase Shift

Explore correlations with $^1S_0$ phse shift from 34 non-implausible interactions

Long-range component in ^{48}Ca, ^{76}Ge



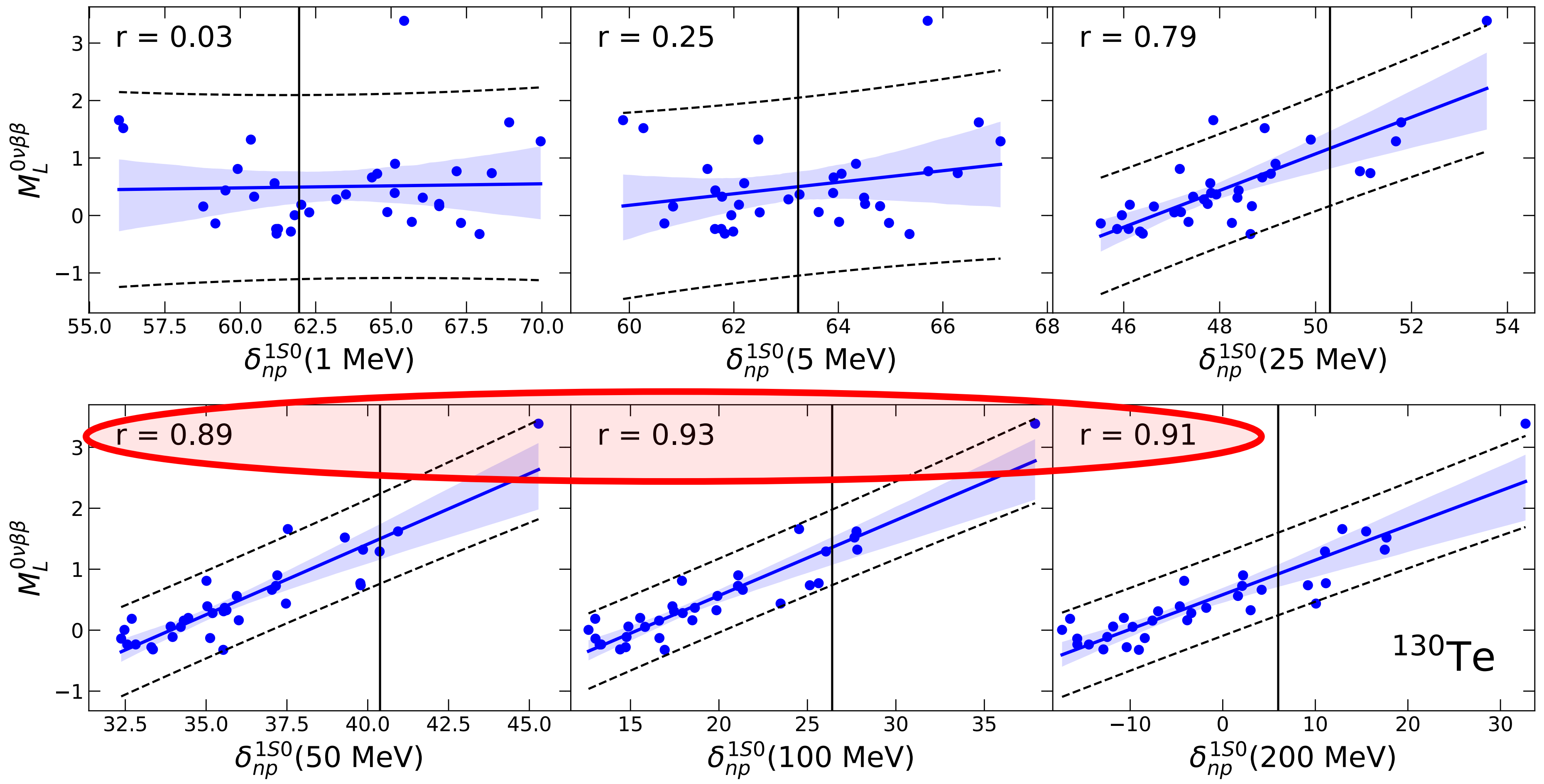
Clear correlation with (measured!) $^1S_0$ phase shift at high scattering energies

TRIUMF

MM-DGP Emulator: Correlation w/ $^1S_0$ Phase Shift

Explore correlations with $^1S_0$ phse shift from 34 non-implausible interactions

Long-range component in ^{48}Ca, ^{76}Ge, ^{130}Te



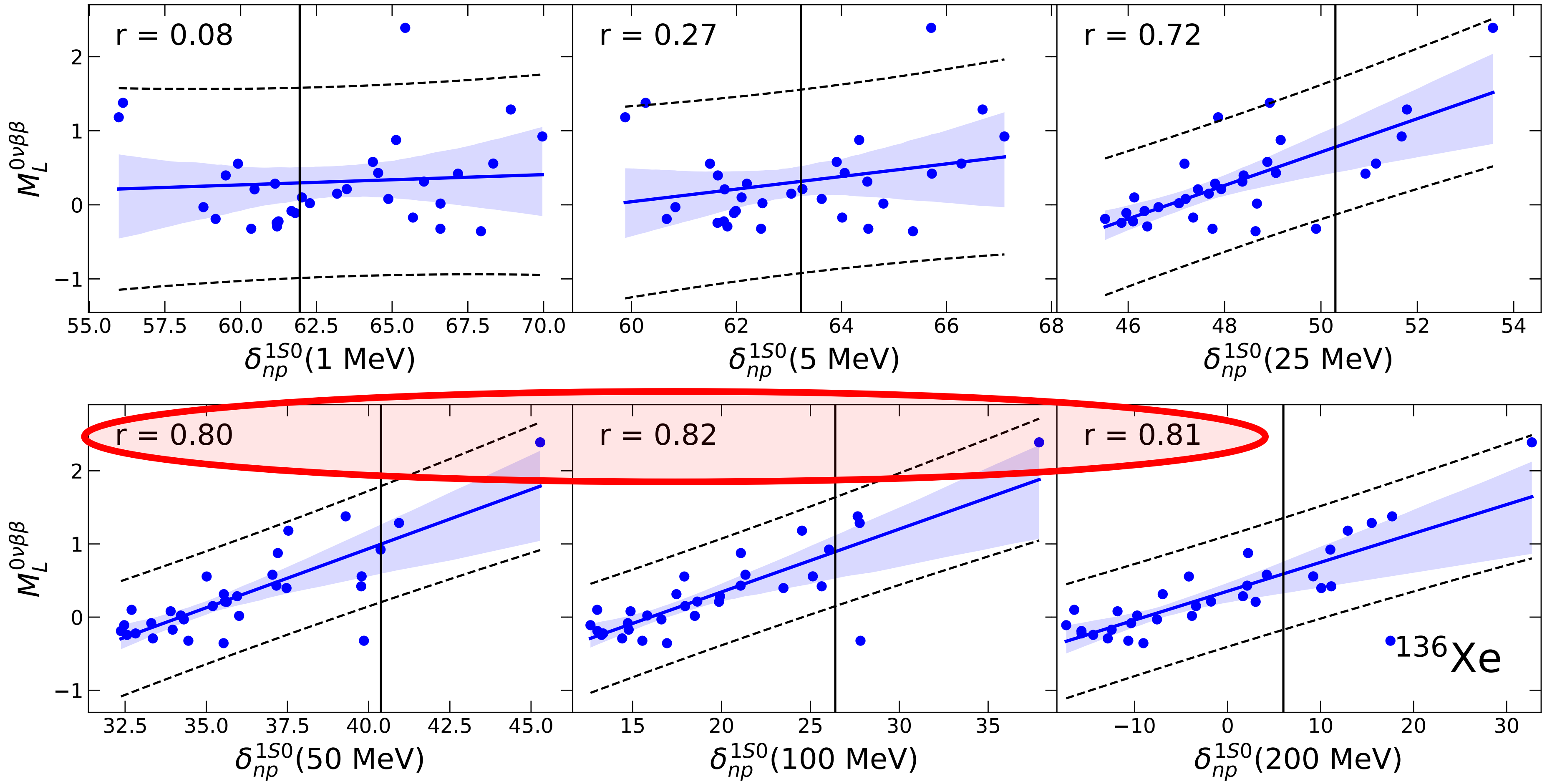
Clear correlation with (measured!) $^1S_0$ phase shift at high scattering energies

TRIUMF

MM-DGP Emulator: Correlation w/ $^1S_0$ Phase Shift

Explore correlations with $^1S_0$ phse shift from 34 non-implausible interactions

Long-range component in ^{48}Ca, ^{76}Ge, ^{130}Te, ^{136}Xe

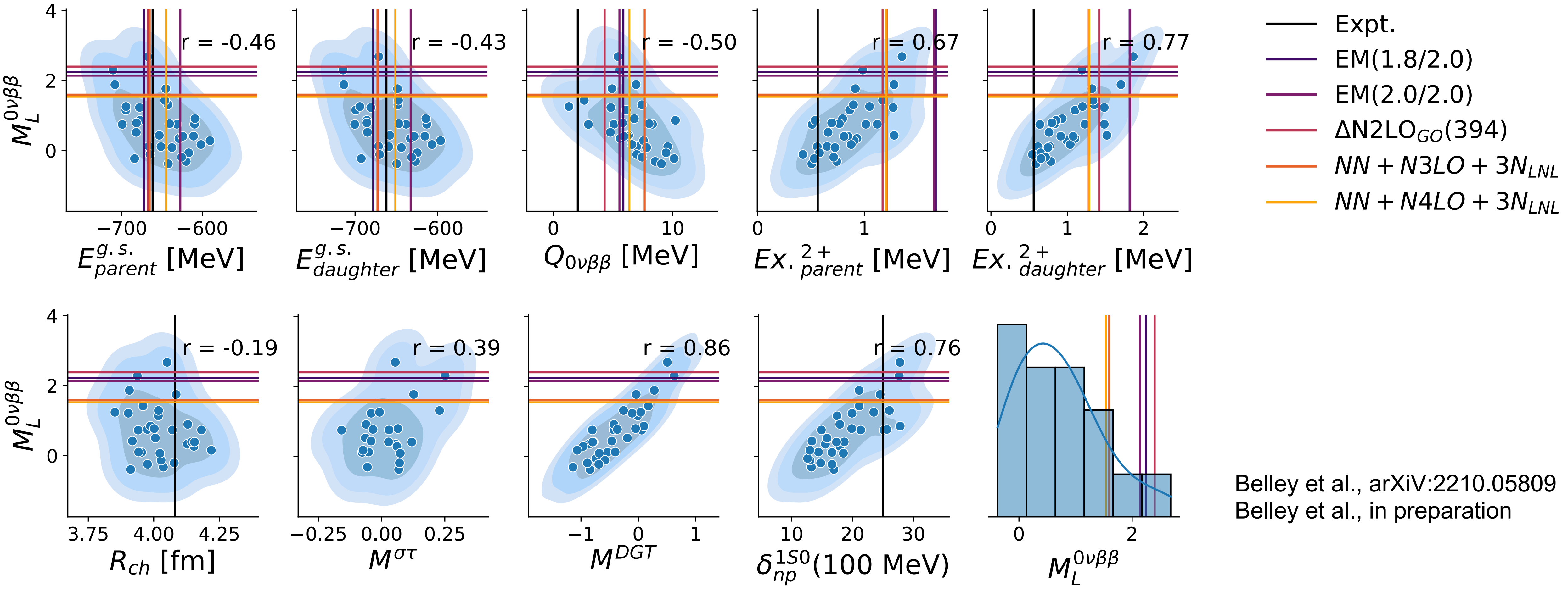


Clear correlation with (measured!) $^1S_0$ phase shift at high scattering energies

Strategy III: Correlation with Structure Observables

Explore correlations with other observables from systematic analysis (34 interactions)

Few clear correlations, except DGT in ^{76}Ge



Belley et al., arXiV:2210.05809
Belley et al., in preparation

Now clear correlation with **measured** $^1S_0$ phase shift!

TRIUMF

Valence-Space IMSRG

Explicitly construct unitary transformation from sequence of rotations

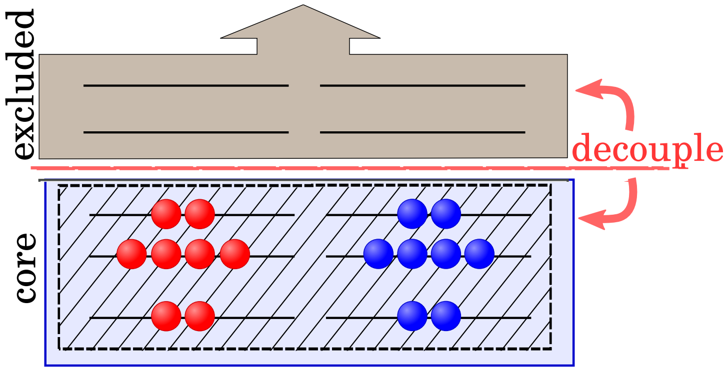
$$U = e^{\Omega} = e^{\eta_n} \dots e^{\eta_1} \qquad \eta = \frac{1}{2} \arctan\left(\frac{2H_{\rm od}}{\Delta}\right) - \text{h.c.}$$

$$\tilde{H} = e^{\Omega} H e^{-\Omega} = H + [\Omega, H] + \frac{1}{2}[\Omega, [\Omega, H]] + \cdots$$

All operators truncated at two-body level IMSRG(2)
IMSRG(3) in progress

Tsukiyama, Bogner, Schwenk, PRC 2012
Morris, Parzuchowski, Bogner, PRC 2015

Step 1: Decouple core



$|\Phi_0\rangle = |^{16}\mathrm{O}\rangle$

Can we achieve accuracy of large-space methods?

$$\langle \tilde{\Psi}_n | P\tilde{H}P \mid \tilde{\Psi}_n\rangle \approx \langle \Psi_i | H | \Psi_i\rangle$$

Valence-Space IMSRG

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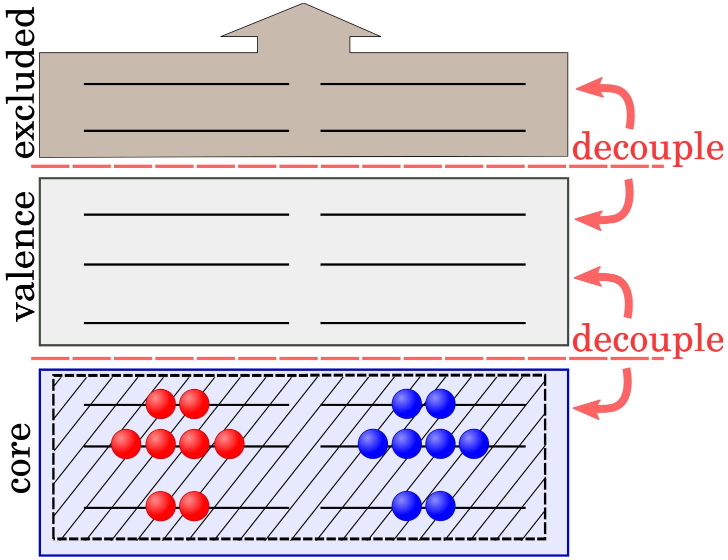

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Step 2: Decouple valence space

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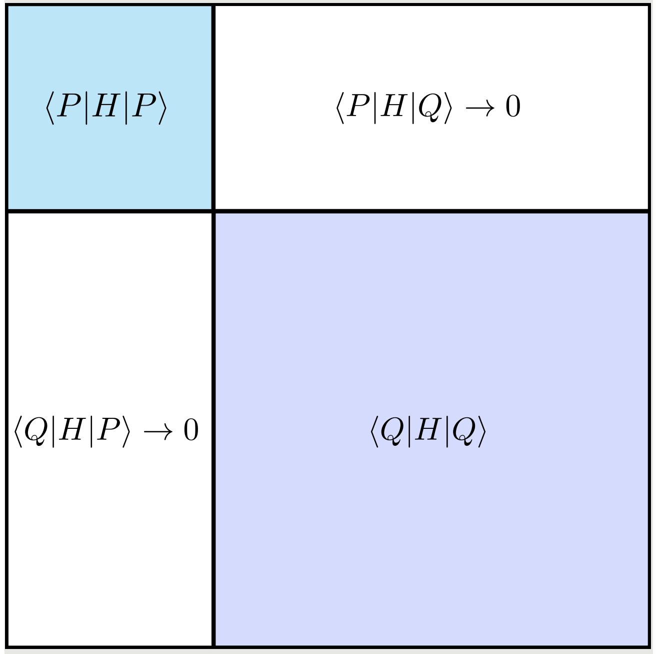

Valence-Space IMSRG

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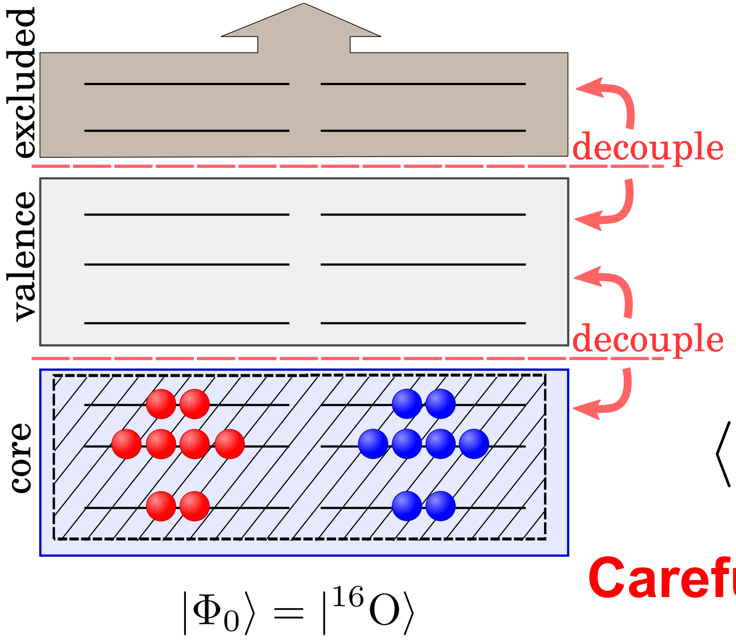
$$U = e^{\Omega} = e^{\eta_n} \dots e^{\eta_1} \qquad \eta = \frac{1}{2} \arctan\left(\frac{2H_{\mathrm{od}}}{\Delta}\right) - \mathrm{h.c.}$$

$$\tilde{H} = e^{\Omega} H e^{-\Omega} = H + [\Omega, H] + \frac{1}{2}[\Omega, [\Omega, H]] + \cdots$$

$$\tilde{\mathcal{O}} = e^{\Omega} \mathcal{O} e^{-\Omega} = \mathcal{O} + [\Omega, \mathcal{O}] + \frac{1}{2}[\Omega, [\Omega, \mathcal{O}]] + \cdots$$

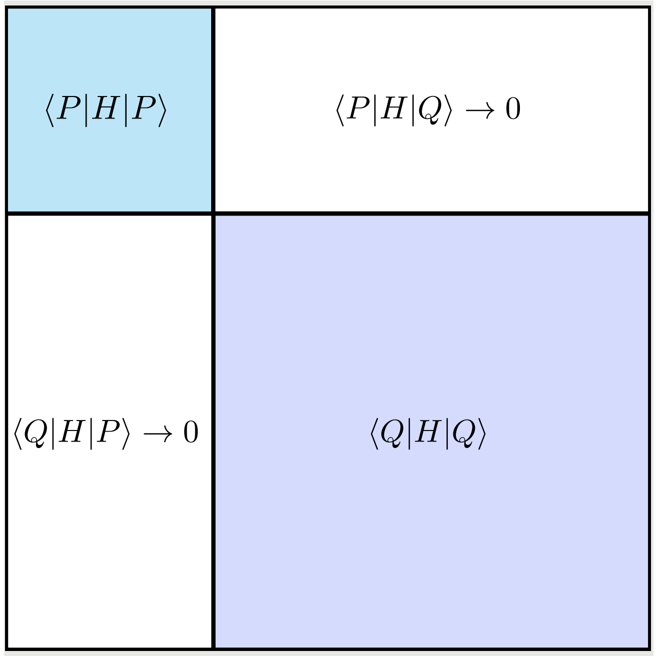


Step 1: Decouple core
Step 2: Decouple valence space
Step 3: Decouple additional operators

$$\langle \tilde{\Psi}_n | P\tilde{H}P \mid \tilde{\Psi}_n \rangle \approx \langle \Psi_i | H | \Psi_i \rangle$$

$$\langle \tilde{\Psi}_n | P\tilde{M}_{0\nu}P \mid \tilde{\Psi}_n \rangle \approx \langle \Psi_i | M_{0\nu} | \Psi_i \rangle$$

Careful benchmarking essential



Strategy IIIb: Sensitivity Analysis

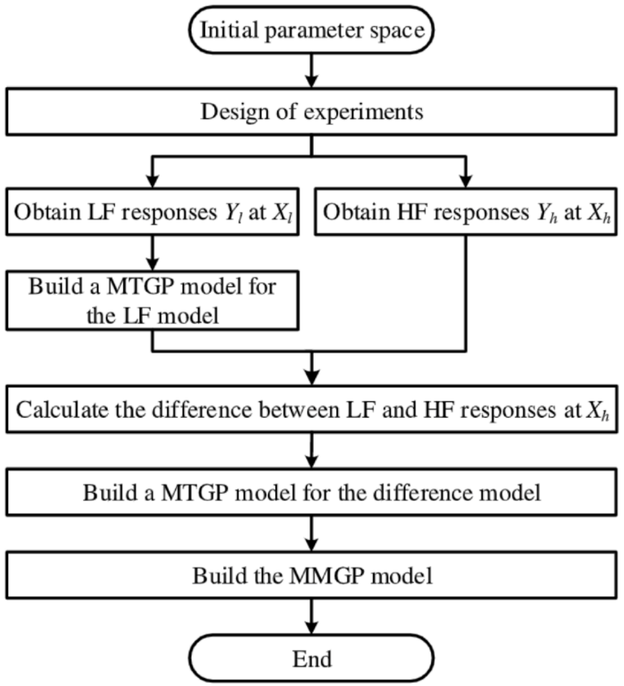
Explore dependence on chiral EFT LECs: requires many samples (as in ^{208}Pb)

Use gaussian processes as an emulator

Multi-Fidelity Gaussian Process: connects few (complicated) high-fidelity data points (eg, full IMSRG) w/ many low-fidelity data points (HF, low e_{max}, etc)

Difference function fit with Gaussian process: predict HF from LF

When relation between LF and HF is complicated, MFGP fails



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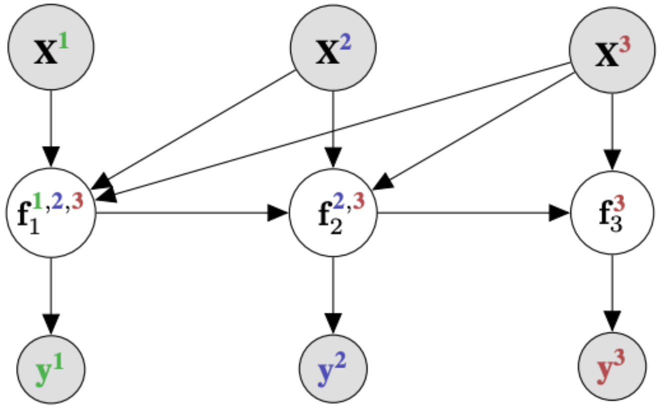
Difference function fit with Gaussian process: predict HF from LF

Deep Gaussian Process: Neural network links multiple GP

Include outputs of previous fidelity as new HF point:
  Improves modeling of difference between LF and HF



Adapted for multi output:
Multi-Output Multi-Fidelity Deep Gaussian Process (MM-DGP)

Belley Pitcher et al., in preparation

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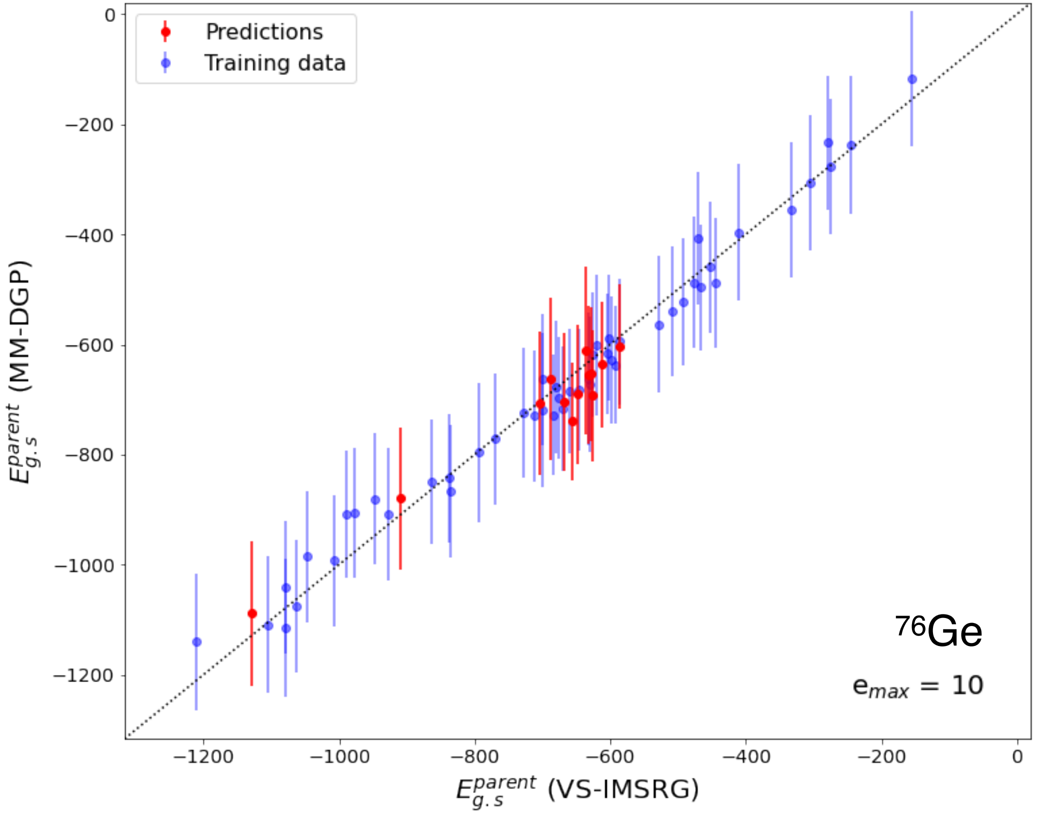
MM-DGP Emulator: Ground-State Energies

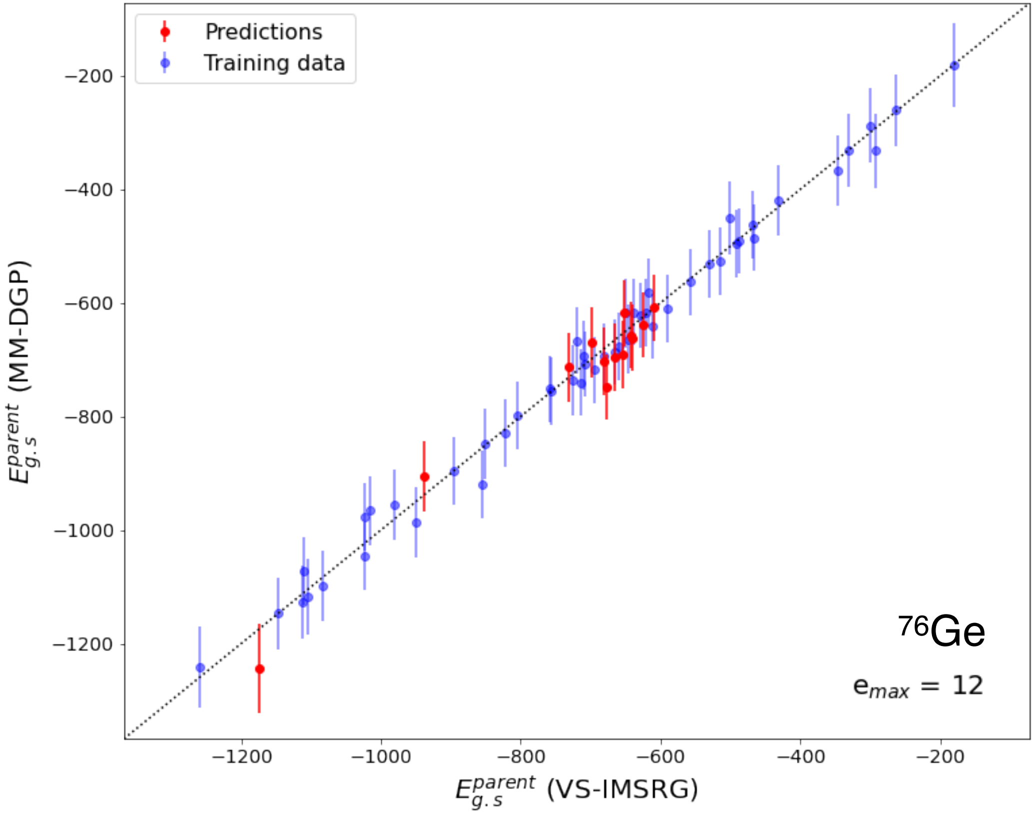
Testing MM-DGP: use delta-full chiral EFT at N2LO

Improved energy predictions with high-fidelity training points

Low-Fidelity



High-Fidelity



Belley, Pitcher et al. in prep.

MM-DGP Emulator: 0νββ-Decay

Testing MM-DGP: use delta-full chiral EFT at N2LO

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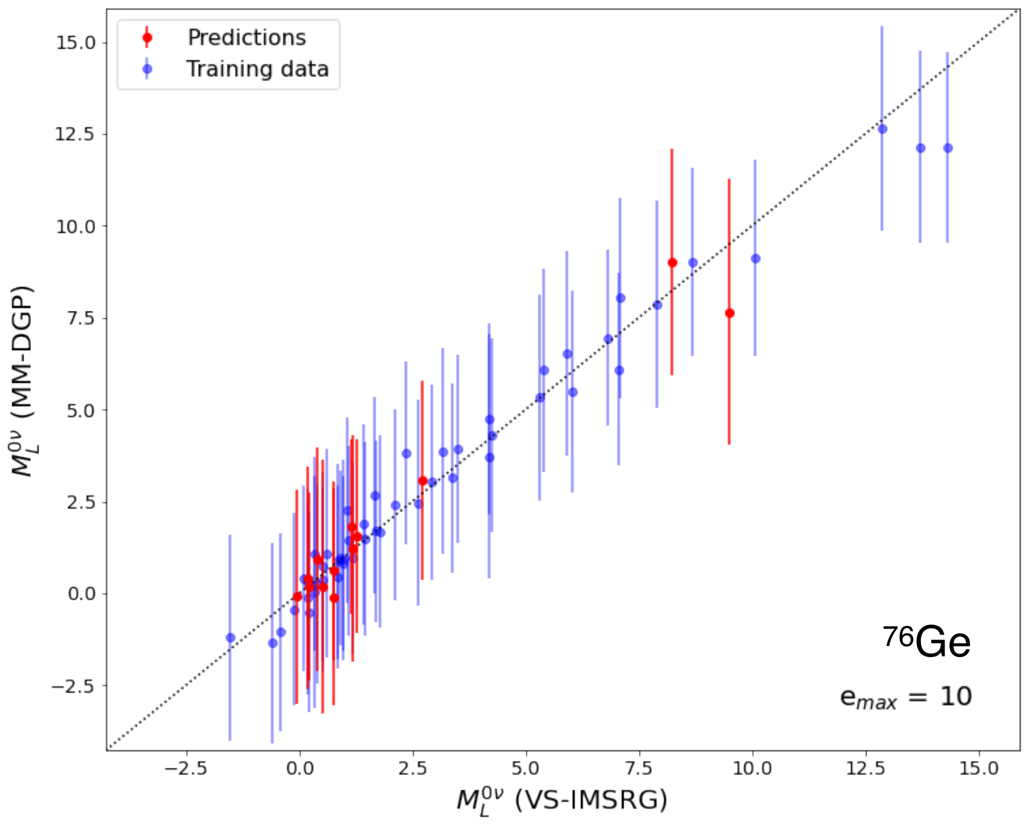
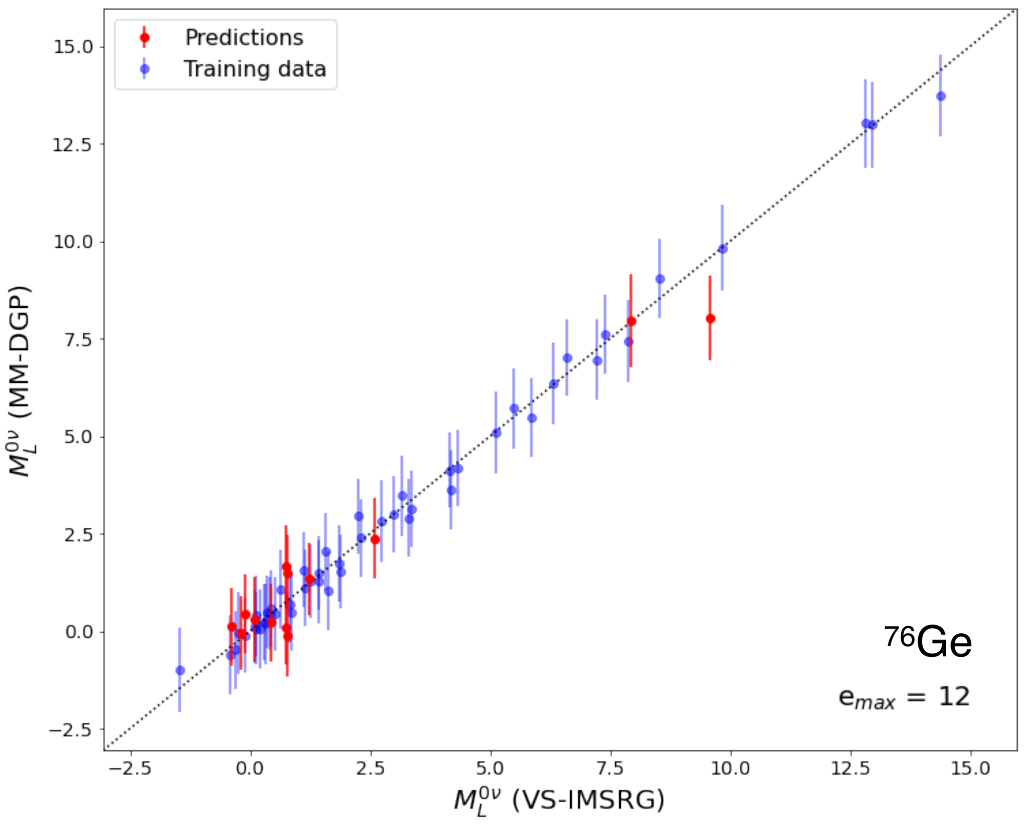
Low-Fidelity



High-Fidelity



Belley, Pitcher et al. in prep.